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                Pre-1988 INPI data added to MARPAT
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        JAN 17
                STN AnaVist, Version 1.1, lets you share your STN AnaVist
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        FEB 21
                 visualization results
                 The IPC thesaurus added to additional patent databases on STN
NEWS 5
        FEB 22
NEWS 6 FEB 22
                Updates in EPFULL; IPC 8 enhancements added
NEWS 7 FEB 27
                New STN AnaVist pricing effective March 1, 2006
NEWS 8 MAR 03
                Updates in PATDPA; addition of IPC 8 data without attributes
NEWS 9
        MAR 22
                EMBASE is now updated on a daily basis
                New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 10
        APR 03
NEWS 11
        APR 03
                Bibliographic data updates resume; new IPC 8 fields and IPC
                 thesaurus added in PCTFULL
                 STN AnaVist $500 visualization usage credit offered
NEWS 12
        APR 04
NEWS 13
        APR 12
                LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 14
        APR 12
                 Improved structure highlighting in FQHIT and QHIT display
                 in MARPAT
NEWS 15
        APR 12
                Derwent World Patents Index to be reloaded and enhanced during
                 second quarter; strategies may be affected
                 CA/CAplus enhanced with 1900-1906 U.S. patent records
NEWS 16
        MAY 10
NEWS 17
        MAY 11
                 KOREAPAT updates resume
NEWS 18
        MAY 19
                Derwent World Patents Index to be reloaded and enhanced
NEWS 19
        MAY 30
                IPC 8 Rolled-up Core codes added to CA/CAplus and
                 USPATFULL/USPAT2
NEWS 20
        MAY 30
                The F-Term thesaurus is now available in CA/CAplus
NEWS 21
        JUN 02
                The first reclassification of IPC codes now complete in
                 INPADOC
NEWS EXPRESS
                 FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
                 CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0jc(jp),
                 AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
                 V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT
                http://download.cas.org/express/v8.0-Discover/
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FILE 'HOME' ENTERED AT 17:01:19 ON 13 JUN 2006

=> file reg COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 12 JUN 2006 HIGHEST RN 887497-01-0 DICTIONARY FILE UPDATES: 12 JUN 2006 HIGHEST RN 887497-01-0

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http://www.cas.org/ONLINE/UG/regprops.html

=> Uploading C:\Program Files\Stnexp\Queries\10540276.str



chain nodes : 6 7 8 11 12 ring nodes : 1 2 3 4 5 chain bonds : 1-11 2-12 4-6 6-7 6-8 ring bonds :

1-2 1-5 2-3 3-4 4-5

exact/norm bonds :

1-2 1-5 1-11 2-3 2-12 3-4 4-5 4-6 6-7 6-8

G1:C,S

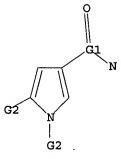
G2:Hy,Cy

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 11:CLASS 12:CLASS

L1 STRUCTURE UPLOADED

=> d l1 L1 HAS NO ANSWERS STR



G1 C,S

G2 Hy,Cy

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 17:01:46 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 3930 TO ITERATE

50.9% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 748

74841 TO 82359

PROJECTED ANSWERS:

782 TO 1732

L2 32 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 17:01:50 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 78731 TO ITERATE

100.0% PROCESSED · 78731 ITERATIONS

1377 ANSWERS

32 ANSWERS

SEARCH TIME: 00.00.02

L3 1377 SEA SSS FUL L1

=> file hcaplus

COST IN U.S. DOLLARS

SINCE FILE . TOTAL

ENTRY SESSION

FULL ESTIMATED COST 166.94 167.15

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Young, Shawquia, Page 4

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=> s 13

L4 29 L3

=> d ed abs ibib hitstr 1-29

L4 ANSWER 1 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 19 May 2006

GI

IV

AB Title compds. [I, II, III; wherein R1 = (un)substituted (cyclo)alkyl, (cyclo)alkenyl, alkynyl, aryl; R2 = H, halo, OH, carboxy, carbamoyl, amino, (un)substituted alkyl, alkoxy; T = independently H, halo, OH, carboxy, carbamoyl, amino, cyano, NO2, alkenyl, alkynyl, cycloalkyl, (un)substituted alkyl, alkoxy; p = 0-5; L = aminocycloalkylideneamino, etc.; Y = bond, CH2, CO2, OCO, SO2, CO, CS, CONH, CSNH, etc.; with

III

provisos; and pharmaceutically acceptable salts, hydrates, or solvates thereof] were prepared as antagonists of melanin concentrating hormone (MCH),

an

endogenous ligand of G-protein coupled receptors (GPCRs). Examples include solution and solid phase general synthetic methods and phys. data for nearly 3400 invention compds. In addition, all exemplified compds. were assayed using high throughput functional screening to detect intracellular Ca2+ concins. for accessing GPCR activation. For instance, reaction of 2,4-dichloro-6-methylpyrimidine with dimethylamine gave 2-chloro-4-(dimethylamino)-6-methylpyrimidine (40%), which was coupled with cis-(4-aminocyclohexyl)carbamic acid tert-Bu ester (60%). Deprotection (72%), amidation, and workup provided the benzamide (IV) ◆TFA. The latter demonstrated MCH antagonist activity with an IC50 value of 7.6 nM. Thus, pharmaceutical compns. comprising I are useful for the prophylaxis or treatment of improving memory function, sleeping and arousal, anxiety, depression, mood disorders, seizure, obesity, diabetes, appetite and eating disorders, cardiovascular disease, hypertension, dyslipidemia, myocardial infarction, binge eating disorders including bulimia, anorexia, mental disorders including manic depression, schizophrenia, delirium, dementia, stress, cognitive disorders, attention deficit disorder, substance abuse disorders, and dyskinesias including Parkinson's disease, epilepsy, and addiction (no data).

ACCESSION NUMBER:

2006:464826 HCAPLUS

TITLE:

Preparation of quinoline, tetrahydroquinazoline, and

pyrimidine derivatives as MCH antagonist for treatment

of CNS disorders

INVENTOR(S):

Sekiguchi, Yoshinori; Kanuma, Yukihiro; Omodera, Katsunori; Busujima, Takeshi; Tran, Thuy-Ahn; Han, Sangdong; Casper, Martin; Brian, A. Kramer; Semple,

Graeme; Zou, Ning

PATENT ASSIGNEE(S):

Taisho Pharmaceutical Co., Ltd., Japan; Arena

Pharmaceutical Inc.

SOURCE:

Jpn. Kokai Tokkyo Koho, 781 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent

LANGUAGE:

Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2006124387	A2	20060518	JP 2005-286311	20050930
PRIORITY APPLN. INFO.:			JP 2004-287659 A	20040930

IT 769183-15-5P 769184-55-6P 769185-93-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(MCH antagonist; preparation of quinolines, quinazolines, and pyrimidines as MCH antagonist for treatment of CNS disorders)

RN 769183-15-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[cis-4-[[4-(dimethylamino)-2-quinolinyl]amino]cyclohexyl]-2-methyl-1,5-diphenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 769184-55-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[cis-4-[[4-(dimethylamino)-2-pyrimidinyl]amino]cyclohexyl]-2-methyl-1,5-diphenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 769185-93-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[cis-4-[[4-(dimethylamino)-5,6,7,8-tetrahydro-2-quinazolinyl]amino]cyclohexyl]-2-methyl-1,5-diphenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 2 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 11 Apr 2006

GI

Pyrrolecarboxamide derivs. (shown as I; other Markush structures for AB pyrrolecarboxamides are defined in the claims; variables defined below; e.g. 1-[4-fluoro-2-(trifluoromethyl)phenyl]-2,5-dimethyl-1H-pyrrole-3carboxylic acid N-[4-(sulfamoyl)phenyl]amide (II)), compns. and methods for modulating the activity of receptors are provided. In particular compds. and compns. are provided for modulating the activity of receptors and for the treatment, prevention, or amelioration of ≥1 symptoms of disease or disorder directly or indirectly related to the activity of the receptors. Semiquant. IC50 values for antagonist activity of 23 examples of I are tabulated and compared to the activity of the Spironolactone control. For I: R1 and R2 = H, halo, cyano, or (un) substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl, heteroaryl, heteroaralkyl, heterocyclyl, or heterocyclylalkyl, or -OR9, -SR9, -N(R9)2, -C(0)OR9 or -C(0)N(R9)2; R3 = H, halo, cyano, (un) substituted alkyl, (un) substituted alkenyl or (un) substituted alkynyl; R4 is H, -C(0)R9, -S(0)2R9, or (un) substituted alkyl, alkenyl or alkynyl, or R4 is (un) substituted cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl or heteroaralkyl; R6 is H or (un) substituted alkyl; R7 is (un) substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, heterocyclyl, heterocyclylalkyl, aryl, aralkyl, heteroaryl or heteroaralkyl; addnl. details are given in the claims. Although the methods of preparation are not claimed, prepns. and/or characterization data for many examples of I are included. For example, II was prepared in 5 steps (50, 37, 62, 64, and 66 % yields, resp.) starting with preparation of 1-[4-fluoro-2-(trifluoromethyl)phenyl]-2,5-dimethyl-1H-pyrrole from 4-fluoro-2-(trifluoromethyl) aniline and 2,5-hexanedione, followed by preparation of the following intermediates: 1-(4-fluoro-2trifluoromethylphenyl) -2,5-dimethyl-1H-pyrrole-3-carboxaldehyde, 1-[4-fluoro-2-(trifluoromethyl)phenyl]-2,5-dimethyl-1H-pyrrole-3carboxylic acid, and 1-[4-fluoro-2-(trifluoromethyl)phenyl]-2,5-dimethyl-1H-pyrrole-3-carbonyl chloride and finally amide formation with sulfanilamide.

ACCESSION NUMBER:

2006:332235 HCAPLUS

DOCUMENT NUMBER:

144:350539

TITLE:

Preparation of pyrrolecarboxamide derivatives as mineralocorticoid receptor antagonists for use against

cancer and other disorders

INVENTOR(S):

Canne Bannen, Lynne; Chen, Jeff; Dalrymple, Lisa Esther; Flatt, Brenton T.; Forsyth, Timothy Patrick; Gu, Xiao-Hu; Mac, Morrison B.; Mann, Larry W.; Mann, Grace; Martin, Richard; Mohan, Raju; Murphy, Brett; Nyman, Michael Charles; Stevens, William C., Jr.;

Wang, Tie-Lin; Wong, Yong; Wu, Jason H.

PATENT ASSIGNEE(S):

SOURCE:

Exelixis, Inc., USA PCT Int. Appl., 477 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent English

LANGUAGE:

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

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PATENT NO.
                        KIND
                                DATE
                                           APPLICATION NO.
                                                                   DATE
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                                                                   -----
     WO 2006012642
                         A2
                                20060202
                                           WO 2005-US26916
                                                                   20050730
         W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
            LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA,
            NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK,
             SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU,
             ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
PRIORITY APPLN. INFO.:
                                           US 2004-592439P
                                                                   20040730
                                            US 2004-592469P
                                                                P 20040730
OTHER SOURCE(S):
                        MARPAT 144:350539
     880779-30-6P, 5-(4-Fluorophenyl)-2-methyl-1-(2-
     trifluoromethylphenyl)-1H-pyrrole-3-carboxylic acid N-(4-
     methylsulfonylphenyl)amide 880779-31-7P, 1,5-Bis(4-fluorophenyl)-
     2-methyl-1H-pyrrole-3-carboxylic acid N-(4-methylsulfonylphenyl)amide
     880779-32-8P, 5-(4-Fluorophenyl)-2-methyl-1-(2-
     trifluoromethylphenyl)-1H-pyrrole-3-carboxylic acid N-(3-methoxy-4-
     sulfamoylphenyl) amide 880779-33-9P,
     5-(4-Fluorophenyl)-2-methyl-1-(2-trifluoromethylphenyl)-1H-pyrrole-3-
     carboxylic acid dimethylamide 880779-73-7P, 4-Methyl-N-[4-
     (methylsulfonyl)phenyl]-1-phenyl-5-[2-(trifluoromethyl)phenyl]-1H-pyrrole-
     3-carboxamide
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (drug candidate; preparation of pyrrolecarboxamide derivs. as
        mineralocorticoid receptor antagonists for use against cancer and other
        disorders)
RN
     880779-30-6 HCAPLUS
CN
     1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-2-methyl-N-[4-
     (methylsulfonyl)phenyl]-1-[2-(trifluoromethyl)phenyl]- (9CI)
                                                                   (CA INDEX
    NAME)
```

RN 880779-31-7 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1,5-bis(4-fluorophenyl)-2-methyl-N-[4-(methylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)

RN 880779-32-8 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[4-(aminosulfonyl)-3-methoxyphenyl]-5-(4-fluorophenyl)-2-methyl-1-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 880779-33-9 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4

1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-N,N,2-trimethyl-1-[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

$$F_3C$$
 Me
 Me_2N-C
 O

RN 880779-73-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 4-methyl-N-[4-(methylsulfonyl)phenyl]-1-phenyl-5[2-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

ANSWER 3 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN L4ED

Entered STN: 30 Dec 2005

GI

The invention provides compns. adapted to enhance reverse cholesterol AB transport in mammals and which are suitable for oral delivery and useful in the treatment and/or prevention of hypercholesterolemia, atherosclerosis and associated cardiovascular diseases. Mediators of reverse cholesterol transport comprise a structure having components A, B and C, where A comprises an acidic moiety having an acidic group or a bioisostere, B comprises an aromatic or lipophilic moiety having at least a portion of HMGCoA reductase inhibitor or an analog, and C comprises a basic moiety having a basic group or bioisostere. An example describes the synthesis of lipophilic group-modified peptide sequence I.TFA based on atorvastatin.

ACCESSION NUMBER: 2005:1354478 HCAPLUS

DOCUMENT NUMBER: 144:88561

TITLE: Preparation of amino acid heterocyclic derivatives for

> treatment of hyperlipidemia and related diseases Sircar, Jagadish C.; Thomas, Richard J.; Khatuya,

Haripada; Nikoulin, Igor

PATENT ASSIGNEE(S): Avanir Pharmaceuticals, USA SOURCE:

PCT Int. Appl., 106 pp.

CODEN: PIXXD2

INVENTOR(S):

DOCUMENT TYPE:

Patent English

LANGUAGE:

Flidi

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

						KIND DATE				APPLICATION NO.						DATE			
	WO 2005123686								WO 2005-US20660						20050609				
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								GR,											
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			MR,	NE,	SN,	TD,	TG												
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IT	872	2406-	24-1	P 87	2406	-25-2	2P 8	7240	5-26	-3P									
	872	406-	27-41	P 87	2406	-28-	5P 8	7240	5-29	-6P									
	872	406-	30-91	P									•						
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	(Th	erap	euti	c use	∍); 1	BIOL	(Bi	olog:	ical	stu	dy);	PRE	P (P:	repai	ratio	on);	USES	3	
	(Us	ses)																	
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	ami	.no-5	-oxo	- (90	CI)	(CA	IND	EX N	AME)										

RN 872406-25-2 HCAPLUS

CN Butanoic acid, 4-[[[4-[[5-[(aminoiminomethyl)amino]-1-oxopentyl]amino]-2-methyl-1,5-diphenyl-1H-pyrrol-3-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

RN 872406-26-3 HCAPLUS

CN Pentanoic acid, 4-(acetylamino)-5-[[4-[[[1-(aminocarbonyl)-4[(aminoiminomethyl)amino]butyl]amino]carbonyl]-5-methyl-1,2-diphenyl-1Hpyrrol-3-yl]amino]-5-oxo- (9CI) (CA INDEX NAME)

RN 872406-27-4 HCAPLUS

CN Pentanoic acid, 5-[[4-[[4-[(aminoiminomethyl)amino]butyl]amino]carbonyl]-5-methyl-1,2-diphenyl-1H-pyrrol-3-yl]amino]-5-oxo- (9CI) (CA INDEX NAME)

RN 872406-28-5 HCAPLUS

CN Benzoic acid, 3-[[[4-[[2-(acetylamino)-5-[(aminoiminomethyl)amino]-1-oxopentyl]amino]-2-methyl-1,5-diphenyl-1H-pyrrol-3-yl]carbonyl]amino]-(9CI) (CA INDEX NAME)

RN 872406-29-6 HCAPLUS

CN Benzoic acid, 3-[[[4-[[5-[(aminoiminomethyl)amino]-1-oxopentyl]amino]-2-methyl-1,5-diphenyl-1H-pyrrol-3-yl]carbonyl]amino]- (9CI) (CA INDEX NAME)

RN 872406-30-9 HCAPLUS

CN Pentanoic acid, 5-[[4-[[[4-(aminoiminomethyl)phenyl]amino]carbonyl]-5-methyl-1,2-diphenyl-1H-pyrrol-3-yl]amino]-5-oxo-(9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 4 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 02 Sep 2005

GI

L4

$$R^{5}$$
 R^{4} R^{2} R^{3} R^{2} R^{2} R^{2} R^{2} R^{2} R^{3} R^{2} R^{2

AB The title compds. I [R1 = substituted alkoxy, sulfonyl, sulfonamide or silanyl; Ra = halo, alkyl or alkoxy; m, n = 0-3; R2 = alkyl, alkoxy, etc; R3 = H, alkyl, alkoxy, etc.; R4 = some carbonyl, etc.; R5 = H or alkyl, and pharmaceutically acceptable salts and solvates thereof], which are active in the CB1 receptor (IC50 < 1 μM) and believed to be selective CB1 antagonists or inverse agonists. were prepared As an example, condensation of Et acetoacetate with 2.2',4'-trichloroacetophenone using NaH as base (37%) followed by cyclization with 4-benzyloxyaniline hydrochloride (39%) gave pyrrole carboxylate II (R = OEt), which was hydrolyzed with NaOH and then coupled with 1-aminopiperidine to afford amide II (R = 1-piperidinylamino). Therefore, I and their pharmaceutical compns. may be used in the treatment of obesity, psychiatric disorders, neurol. disorders and so on.

ACCESSION NUMBER: 2005:962204 HCAPLUS

DOCUMENT NUMBER: 143:248281

TITLE: Preparation of pyrrole-3-carboxamide derivatives for

the treatment of obesity and other diseases

Bjornse, Magnus; Cheng, Leifeng; Elebring, Thomas; INVENTOR(S):

Boije, Anna Maria; Alstermark Lindstedt, Eva-Lotte

PATENT ASSIGNEE(S): Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

	LY ACC.			NT :	1													
			KIND DATE				APPLICATION NO.					DATE						
	WO 2005080328			A1 20050901			WO 2005-GB588											
٠	W:	ΑE,	AG,	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BW,	BY,	ΒZ,	CA,	CH,	
		CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,	
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RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP																		
(Preparation); RACT (Reactant or reagent); USES (Uses)																		
(drug candidate; preparation of pyrrolecarboxamides for treatment of obesity																		
		othe							-									
RN	863332	-15-4	HC.	APLU	S													
CN	1H-Pyr																	
	(pheny)	lmeth	oxy)	phen	yl] -1	N-1-	pipe:	ridi	nyl-	(9C)	I)	(CA	INDE	K NA	ME)			

TT 863332-18-7P, 4-[5-(2,4-Dichlorophenyl)-2-methyl-3-[[(piperidin-1yl)amino]carbonyl]-1H-pyrrol-1-yl]phenyl trifluoromethanesulfonate 863332-22-3P, 5-(2,4-Dichlorophenyl)-2-methyl-N-(piperidin-1-yl)-1-[4-(3,3,3-trifluoropropoxy)phenyl]-1H-pyrrole-3-carboxamide 863332-23-4P, 4-[5-(2,4-Dichlorophenyl)-2-methyl-3-[[(piperidin-1yl)amino]carbonyl]-1H-pyrrol-1-yl]phenyl butane-1-sulfonate 863332-25-6P, 5-(2,4-Dichlorophenyl)-2-methyl-1-[4-(trimethylsilanyl)phenyl]-1H-pyrrole-3-carboxylic acid N-(piperidin-1-yl)amide 863332-26-7P, 4-[5-(2,4-Dichlorophenyl)-2-methyl-3-[[(piperidin-1-yl)amino]carbonyl]-1H-pyrrol-1-yl]phenyl propane-1-sulfonate RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (drug candidate; preparation of pyrrolecarboxamides for treatment of obesity and other diseases) RN863332-18-7 HCAPLUS CN Methanesulfonic acid, trifluoro-, 4-[5-(2,4-dichlorophenyl)-2-methyl-3-[(1piperidinylamino)carbonyl]-1H-pyrrol-1-yl]phenyl ester (9CI) (CA INDEX NAME)

RN 863332-22-3 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dichlorophenyl)-2-methyl-N-1-piperidinyl1-[4-(3,3,3-trifluoropropoxy)phenyl]- (9CI) (CA INDEX NAME)

RN 863332-23-4 HCAPLUS

CN 1-Butanesulfonic acid, 4-[5-(2,4-dichlorophenyl)-2-methyl-3-[(1-piperidinylamino)carbonyl]-1H-pyrrol-1-yl]phenyl ester (9CI) (CA INDEX NAME)

RN 863332-25-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dichlorophenyl)-2-methyl-N-1-piperidinyl-1-[4-(trimethylsilyl)phenyl]- (9CI) (CA INDEX NAME)

RN 863332-26-7 HCAPLUS

CN 1-Propanesulfonic acid, 4-[5-(2,4-dichlorophenyl)-2-methyl-3-[(1-piperidinylamino)carbonyl]-1H-pyrrol-1-yl]phenyl ester (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 19 Aug 2005

GΙ

AB The invention provides pyrrole-containing compds. and methods of use thereof. Kits and pharmaceutical compns. comprising the pyrrole compds. of the invention are also provided. The compds. and compns. disclosed herein are preferably used in the treatment of neurodegenerative diseases, cardiovascular diseases, proliferative diseases, neuroinflammatory disorders, vascular disorders with an inflammatory component, and visual disorders. In particular, methods and compns. for the treatment of stroke are disclosed herein. Preparation of compds. of the invention, e.g. I, is included.

ACCESSION NUMBER:

2005:824494 HCAPLUS

DOCUMENT NUMBER:

143:206476

TITLE:

Pyrrole compounds for use in the treatment of stroke

and other conditions

INVENTOR(S): Lockhart, David J.; Patel, Hitesh K.; Milanov, Zdravko

V.; Mehta, Shamal Anil; Zarrinkar, Patrick Parvis; Biggs, William H.; Ciceri, Pietro; Fabian, Miles A.;

Treiber, Daniel Kelly

PATENT ASSIGNEE(S): Ambit Biosciences Corp., USA

SOURCE: U.S. Pat. Appl. Publ., 93 pp., Cont.-in-part of U.S.

Ser. No. 848,584.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 5

PATENT INFORMATION:

PATENT NO.	KIND	DATE	AP	PLICATION NO.		DATE
					-	
US 2005182125	A1	20050818	US	2004-989995		20041115
US 2004259880	A1	20041223	US	2004-848584		20040518
PRIORITY APPLN: INFO.:			US	2003-471425P	P	20030516
			US	2003-480289P	P	20030620
·			US	2003-480475P	P	20030620
			US	2003-488172P	P	20030716
			US	2003-488178P	P	20030716
			US	2003-516610P	P	20031030
			US	2003-516616P	P	20031030
			US	2003-516651P	P	20031030
			US	2004-848584	A2	20040518

OTHER SOURCE(S): MARPAT 143:206476

IT 811864-73-0

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pyrrole compds. for use in treatment of stroke and other conditions)

RN 811864-73-0 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-2-(1-methylethyl)-1-(4-methylphenyl)-N,4-diphenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 6 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 24 Dec 2004

AB The invention provides pyrrole-containing compds. and methods of use thereof. Kits and pharmaceutical compns. comprising the pyrrole compds. of the invention are also provided. The compds. and compns. disclosed herein are preferably used in the treatment of neurodegenerative diseases, cardiovascular diseases, proliferative diseases, and visual disorders. In

02/08/2006,10540276.trn particular, methods and compns. for the treatment of stroke are disclosed herein. The compds. described herein are useful in the treatment of various diseases; in particular diseases in which modulation of phosphodiesterase 6, quinone reductase 2, and/or calbindin-2 is desired. 2004:1127333 HCAPLUS ACCESSION NUMBER: DOCUMENT NUMBER: 142:69218 Pyrrole compounds and uses thereof TITLE: Lockhart, David J.; Patel, Hitesh K.; Milanov, Zdravko INVENTOR(S): V.; Mehta, Shamal Anil; Zarrinkar, Patrick Parvis; Biggs, William H., III; Ciceri, Pietro; Fabian, Miles A.; Treiber, Daniel Kelly PATENT ASSIGNEE(S): Ambit Biosciences Corporation, USA SOURCE: PCT Int. Appl., 142 pp. CODEN: PIXXD2 DOCUMENT TYPE: Patent LANGUAGE: English FAMILY ACC. NUM. COUNT: PATENT INFORMATION: PATENT NO. DATE APPLICATION NO. KIND DATE -------------------WO 2004110998 A1 20041223 WO 2004-US15444 20040517 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,

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SN, TD, TG
    US 2004242673
                         A1
                               20041202
                                           US 2004-847897
                                                                  20040517
    US 2004248972
                        A1
                               20041209
                                           US 2004-848515
                                                                  20040517
    US 2004248957
                               20041209
                                           US 2004-848521
                        A1
                                                                  20040517
                                           AU 2004-247627
    AU 2004247627
                               20041223
                        A1
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    CA 2523808
                               20041223
                                           CA 2004-2523808
                        AA
                                                                 20040517
    EP 1636183
                        A1
                               20060322
                                           EP 2004-752457
                                                                 20040517
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK
PRIORITY APPLN. INFO.:
                                           US 2003-471425P
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                                           US 2003-480289P
                                                              P 20030620
                                           US 2003-480475P
                                                              P 20030620
                                           US 2003-488172P
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                                           US 2003-488178P
                                                              P 20030716
                                           US 2003-516610P
                                                              P 20031030
                                           US 2003-516616P
                                                              P 20031030
                                           US 2003-516651P
                                                              P 20031030
                                           WO 2004-US15444
                                                              W 20040517
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OTHER SOURCE(S): MARPAT 142:69218 811864-73-0

> RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pyrrole compds. for disease treatment by modulation of phosphodiesterase 6 subunits and binding to GTPase and quinone reductase 2 and calbindin-2)

RN811864-73-0 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-2-(1-methylethyl)-1-(4methylphenyl) -N, 4-diphenyl- (9CI) (CA INDEX NAME)

REFERENCE COUNT: THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS 1 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4ANSWER 7 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 12 Nov 2004

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. Q-L-Y-R1 [Q = Q1, H2NC(:NH); wherein R2 = NHNH2, NHNHBoc, (un) substituted NH2, morpholino, 4-acetyl-piperazinyl, 4-phenylpiperazinyl; R1 = each (un)substituted C1-16 alkyl, C2-8 alkenyl, C2-4 alkynyl, C3-6 cycloalkyl, C3-6 cycloalkenyl, carbocyclyl, carbocyclic alkyl, or heterocyclyl; L = each Q2-Q6 or its cis- or trans-isomer, Q7-Q16; R4 = H, C1-3 alkyl; R5 = H, each (un)substituted carbocyclic aryl or C1-3 alkyl; Y = SO2, CO, a single bond, CH2] or salts thereof are prepared These compds. are MCH receptor antagonists and used for regulating orphan G protein-coupled receptor SLC-1 and for the prevention and/or treatment of obesity, obesity-related diseases, anxiety, or depression. Thus, hydrogenolysis of benzyl cis-[[4-(4-dimethylaminoquinazolin-2ylamino)cyclohexyl]methyl]carbamate over 5% Pd-C in MeOH at 50° under H atmospheric for 3 days gave a solution of

cis-[[4-(4-dimethylaminoguinazolin-

2-ylamino)cyclohexyl]methyl]amine in MeOH which underwent reductive alkylation with 4-bromo-2-trifluoromethoxybenzaldehyde and NaBH(OAc)3 in AcOH/CH2Cl2 to give, after purification using HPLC and treatment with 4 N HCl/EtOAc, compound (I).2HCl. In a high throughput function screen for identifying lead compds., I.2HCl inhibited the human MCH-induced cellular Ca2+ flux with IC50 of 6 μg/mL.

ACCESSION NUMBER: 2004:963181 HCAPLUS

DOCUMENT NUMBER: 141:379941

TITLE: Preparation of quinazoline-2,4-diamines as melanin

concentrating hormone (MCH) receptor antagonists Sekiguchi, Yoshikatsu; Kanuma, Yukihiro; Omodera,

INVENTOR(S):

Katsunori; Tran, Thuy-ahn; Kramer, Bryan Aubrey;

Beeley, Nigel Robert Arnold

Taisho Pharmaceutical Co., Ltd., Japan PATENT ASSIGNEE(S):

SOURCE:

Jpn. Kokai Tokkyo Koho, 988 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent Japanese

LANGUAGE:

Ja.

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE -**--**--------------JP 2004315511 A2 20041111 JP 2004-95046 20040329 PRIORITY APPLN. INFO.: JP 2003-93418 A 20030331

OTHER SOURCE(S):

MARPAT 141:379941

IT 509143-54-8P 510743-47-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of quinazoline derivs. as melanin-concentrating hormone (MCH) receptor $\dot{}$

RN 509143-54-8 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[cis-4-[[4-(dimethylamino)-2-quinazolinyl]amino]cyclohexyl]-2-methyl-1,5-diphenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 510743-47-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[[cis-4-[[4-(dimethylamino)-2-quinazolinyl]amino]cyclohexyl]methyl]-2-methyl-1,5-diphenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.

L4 ANSWER 8 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Entered STN: 08 Oct 2004

ED GI

$$(T) p \xrightarrow{R^2} (T) p \xrightarrow{R^2} N \xrightarrow{L^{Y}_{R^1}} I$$

AB Title compds. I, II, and III [wherein R1 = (un)substituted (cyclo)alkyl, (cyclo)alkenyl, alkynyl, aryl; R2 = H, halo, OH, carboxy, carbamoyl, amino, (un)substituted alkyl, alkoxy; T = independently H, halo, OH, carboxy, carbamoyl, amino, cyano, NO2, alkenyl, alkynyl, cycloalkyl, (un)substituted alkyl, alkoxy; p = 0-5; L = aminocycloalkylideneamino, etc.; Y = bond, CH2, CO2, OCO, SO2, CO, CS, CONH, CSNH, etc.; with provisos; and pharmaceutically acceptable salts, hydrates, or solvates thereof] were prepared as antagonists of melanin concentrating hormone (MCH),

IV

an

endogenous ligand of G-protein coupled receptors (GPCRs). Examples include solution and solid phase general synthetic methods and phys. data for nearly 3400 invention compds. In addition, all exemplified compds. were assayed using high throughput functional screening to detect intracellular Ca2+ concns. for accessing GPCR activation. For instance, reaction of 2,4-dichloro-6-methylpyrimidine with dimethylamine gave 2-chloro-4-(dimethylamino)-6-methylpyrimidine (40%), which was coupled with cis-(4-aminocyclohexyl)carbamic acid tert-Bu ester (60%). Deprotection (72%), amidation, and workup provided the benzamide IV-TFA. The latter demonstrated MCH antagonist activity with an IC50 value of 7.6 nM. Thus, pharmaceutical compns. comprising I are useful for the prophylaxis or treatment of improving memory function, sleeping and arousal, anxiety, depression, mood disorders, seizure, obesity, diabetes, appetite and eating disorders, cardiovascular disease, hypertension, dyslipidemia, myocardial infarction, binge eating disorders including bulimia, anorexia, mental disorders including manic depression, schizophrenia, delirium, dementia, stress, cognitive disorders, attention deficit disorder, substance abuse disorders, and dyskinesias including Parkinson's disease, epilepsy, and addiction (no data). This is part I of three in a series covering the patent.

ACCESSION NUMBER:

2004:822842 HCAPLUS

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DOCUMENT NUMBER:
                         141:314346
TITLE:
                         Preparation of quinoline, tetrahydroquinazoline, and
                         pyrimidine derivatives as MCH antagonist for treatment
                         of CNS disorders
INVENTOR(S):
                         Sekiguchi, Yoshinori; Kanuma, Kosuke; Omodera,
                         Katsunori; Busujima, Tsuyoshi; Tran, Thuy-Anh; Han,
                         Sangdon; Casper, Martin; Kramer, Bryan A.; Semple,
                         Graeme; Zou, Ning
PATENT ASSIGNEE(S):
                         Taisho Pharmaceutical Co. Ltd., Japan; Arena
                         Pharmaceuticals, Inc.
SOURCE:
                         Eur. Pat. Appl., 586 pp.
                         CODEN: EPXXDW
DOCUMENT TYPE:
                         Patent
LANGUAGE:
                         English
FAMILY ACC. NUM. COUNT:
PATENT INFORMATION:
     PATENT NO.
                        KIND
                               DATE
                                          APPLICATION NO.
                                                                  DATE
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     EP 1464335
                         A2
                                20041006 EP 2004-7651
                                                                   20040330
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     US 2005197350
                         A1
                                20050908 US 2004-812075
                                                                  20040330
     AU 2004226049
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                         A1
                                20041014
                                                                   20040331
     CA 2518913
                         AA
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                                                                   20040331
     WO 2004087669
                         A1
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             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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     JP 2004300156
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                         Α
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                                                                   20051027
PRIORITY APPLN. INFO.:
                                           US 2003-458530P
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                                           US 2003-495911P
                                                               P 20030819
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                                                               P 20031009
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                                                               P 20031216
                                           WO 2004-JP4624
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OTHER SOURCE(S):
                        MARPAT 141:314346
     769183-15-5P, N-[cis-4-[[4-(Dimethylamino)quinolin-2-
    yl]amino]cyclohexyl]-2-methyl-1,5-diphenyl-1H-pyrrole-3-carboxamide
     769184-55-6P, N-[cis-4-[[4-(Dimethylamino)pyrimidin-2-
    yl]amino]cyclohexyl]-2-methyl-1,5-diphenyl-1H-pyrrole-3-carboxamide
     769185-93-5P, N-[cis-4-[[4-(Dimethylamino)-5,6,7,8-
     tetrahydroquinazolin-2-yl]amino]cyclohexyl]-2-methyl-1,5-diphenyl-1H-
    pyrrole-3-carboxamide
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
        (MCH antagonist; preparation of quinolines, quinazolines, and pyrimidines as
       MCH antagonist for treatment of CNS disorders)
RN
    769183-15-5 HCAPLUS
     1H-Pyrrole-3-carboxamide, N-[cis-4-[[4-(dimethylamino)-2-
CN
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quinolinyl]amino]cyclohexyl]-2-methyl-1,5-diphenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 769184-55-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[cis-4-[[4-(dimethylamino)-2-pyrimidinyl]amino]cyclohexyl]-2-methyl-1,5-diphenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 769185-93-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[cis-4-[[4-(dimethylamino)-5,6,7,8-tetrahydro-2-quinazolinyl]amino]cyclohexyl]-2-methyl-1,5-diphenyl- (9CI) (CA INDEX NAME)

Relative stereochemistry.

- L4 ANSWER 9 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
- ED Entered STN: 19 Aug 2004
- AB A process for the preparation of a stable dispersion of solid particles, in an aqueous medium comprises combining a first solution comprising a substantially water-insol. pyrrolecarboxamide, a water-miscible organic solvent and an inhibitor with an aqueous phase comprising water and optionally a stabilizer.

The solid particles comprising the inhibitor and the water-insol. substance are precipitated and he water-miscible organic solvent is removed. Also

claimed are stable dispersions obtainable by the process, solid particles obtainable by the process and the use of such particles. The process provides a dispersion of solid particles in an aqueous medium, which particles exhibit reduced or substantially no particle growth mediated by Ostwald ripening. The process is particularly suitable for the preparation of small (sub-micron) aqueous dispersions of a substantially water-insol. active substance. Thus, a solution of 1-{[1-(4-chlorophenyl)-5-(2,4-dichlorophenyl)-2-methyl-1H-pyrrol-3-yl]carbonyl}piperidine (90 mM) and 10.0 mg/mL Miglyol 812N in dimethylacetamide was prepared and 0.1 mL this solution was added rapidly to an 0.8-mL aqueous solution containing 0.2% polyvinylpyrrolidone and

 $\,$ mM sodium dodecyl sulfate. The aqueous solution was sonicated during the addition

of the organic solution \bar{n} This resulted in the precipitation of particles with a mean

size of 126 nm. No increase in particle size was observed over a period of 2 h at 20°. The synthesis of pyrrolecarboxamides is given.

ACCESSION NUMBER:

2004:675653 HCAPLUS

DOCUMENT NUMBER:

141:195288

TITLE:

0.25

Aqueous dispersions comprising stable nanoparticles of a water-insoluble pyrrolecarboxamide and medium-chain

triglyceride excipients

INVENTOR(S):

Lindfors, Lennart

PATENT ASSIGNEE(S):

Astrazeneca AB, Swed.; Astrazeneca UK Limited

SOURCE:

PCT Int. Appl., 54 pp. CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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PATENT NO.
                       KIND
                              DATE
                                         APPLICATION NO.
                                                                DATE
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    WO 2004069227
                              20040819 WO 2004-GB402
                        A1
                                                                20040202
            AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
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            MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN,
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    EP 1592404
                        A1
                              20051109
                                          EP 2004-707263
                                                                20040202
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
PRIORITY APPLN. INFO.:
                                          GB 2003-2671
                                                        A 20030206
                                          WO 2004-GB402
                                                            W 20040202
OTHER SOURCE(S):
                       MARPAT 141:195288
    723303-38-6P 723303-39-7P 723303-40-0P
    723303-41-1P 723303-42-2P 723303-43-3P
    723303-44-4P 723303-45-5P 723303-46-6P
    723303-47-7P 723303-49-9P 723303-51-3P
    723303-53-5P 723303-55-7P 723303-57-9P
    723303-60-4P 723303-62-6P
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
    (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
    (Uses)
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(aqueous dispersions comprising stable nanoparticles of water-insol. pyrrolecarboxamide and medium-chain triglyceride excipients)

RN 723303-38-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-methyl-N,1,5-triphenyl- (9CI) (CA INDEX NAME)

RN 723303-39-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-2-methyl-N,5-diphenyl- (9CI) (CA INDEX NAME)

RN 723303-40-0 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-methoxyphenyl)-2-methyl-N,5-diphenyl- (9CI) (CA INDEX NAME)

RN 723303-41-1 HCAPLUS

Young, Shawquia, Page 30

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dichlorophenyl)-2-methyl-N,1-diphenyl-(9CI) (CA INDEX NAME)

RN 723303-42-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-5-(2,4-dichlorophenyl)-2-methyl-N-phenyl- (9CI) (CA INDEX NAME)

RN 723303-43-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dichlorophenyl)-1-(4-methoxyphenyl)-2-methyl-N-phenyl- (9CI) (CA INDEX NAME)

RN 723303-44-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dimethoxyphenyl)-2-methyl-N,1-diphenyl-(9CI) (CA INDEX NAME)

Young, Shawquia, Page 31

RN 723303-45-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-5-(2,4-dimethoxyphenyl)-2-methyl-N-phenyl- (9CI) (CA INDEX NAME)

RN 723303-46-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dimethoxyphenyl)-1-(4-methoxyphenyl)-2-methyl-N-phenyl- (9CI) (CA INDEX NAME)

RN 723303-47-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-methyl-1,5-diphenyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-49-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-2-methyl-5-phenyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-51-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-methoxyphenyl)-2-methyl-5-phenyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-53-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dichlorophenyl)-2-methyl-1-phenyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-55-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-5-(2,4-dichlorophenyl)-2methyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-57-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dichlorophenyl)-1-(4-methoxyphenyl)-2-methyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-60-4 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-5-(2,4-dimethoxyphenyl)-2methyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-62-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dimethoxyphenyl)-1-(4-methoxyphenyl)-2methyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

L4 ANSWER 10 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 23 Jul 2004 GI

$$R^{1}$$
 $N-R^{2}$
 R^{6}
 R^{5}
 R^{1}
 R^{3}
 R^{7}
 R^{4}

AB The invention relates to a preparation of novel 2-(thiazol-4-yl)pyrrole derivs. of formula I [wherein: R1 is H or alkyl; R2 is H, alkyl, alkenyl, or alkoxy-alkyl, etc.; R3 is alkyl, alkenyl, alkoxy-alkyl, or di-phenyl-alkyl, etc.; R4 is (un)substituted (cyclo)alkyl, alkoxycarbonyl, or 5- or 6-membered heterocycle; R5 and R6 are independently selected from

H, alkyl, halogen, or fluorinated methyl; R7 is H, alkyl, or halogen], useful as CB1 receptor antagonists. The invention compds. are useful for the treatment and/or prophylaxis of diseases which are associated with the modulation of CB1 receptors. For instance, 2-(thiazol-4-yl)pyrrole derivative II (IC50 < 2 μM) was prepared using aminomethylcyclohexane, butylamine, and 2-chlorothiobenzamide (no yield data, example 7).

ACCESSION NUMBER:

2004:589547 HCAPLUS

DOCUMENT NUMBER:

141:140427

TITLE:

A preparation of novel 2-(thiazol-4-yl)pyrrole derivatives, useful as CB1 receptor antagonists

INVENTOR(S):

Guba, Wolfgang; Haap, Wolfgang; Marty, Hans Peter;

Narquizian, Robert

PATENT ASSIGNEE(S):

F. Hoffmann-La Roche A.-G., Switz.

SOURCE:

PCT Int. Appl., 235 pp.

CODEN: PIXXD2 Patent

DOCUMENT TYPE: LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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            OM, PG; PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
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PRIORITY APPLN. INFO.:
                                                              A 20030102
                                           EP 2003-2
                                           WO 2003-EP14721
                                                              W 20031222
OTHER SOURCE(S):
                        MARPAT 141:140427
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726179-20-0P 726179-42-6P 726179-98-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(preparation of novel thiazolylpyrrole derivs., useful as CB1 receptor antagonists)

RN 726179-20-0 HCAPLUS

1H-Pyrrole-3-carboxamide, N-butyl-1-(4-chlorophenyl)-5-[2-(4-CN methoxyphenyl)-4-thiazolyl]-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & C1 \\ \hline \\ Me & N \\ \hline \\ N & S \\ \\ N & S \\ \hline \\$$

RN 726179-42-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-butyl-1-(2,3-dihydro-1H-inden-2-yl)-5-[2-(4-methoxyphenyl)-4-thiazolyl]-2-methyl- (9CI) (CA INDEX NAME)

RN 726179-98-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-cyclohexyl-N-(cyclopropylmethyl)-5-[2-(4-methoxyphenyl)-4-thiazolyl]-2-methyl-(9CI) (CA INDEX NAME)

L4 ANSWER 11 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 15 Jul 2004

GI

$$R^3$$
 $X-Y-NR^4R^5$
 R^2
 R^6
 R^1
 R^1

AB Title compds. I [wherein R1, R2 = independently (un) substituted Ph, thienyl, pyridyl; R3 = H, (amino) alkyl, alkoxymethyl, trifluoromethyl, etc.; R4, R5 = independently (un) substituted (amino) alkyl, non-aromatic carbocyclic, cycloalkylalkyl, etc.; R6 = H, (hydroxy) alkyl, alkoxymethyl, carbamoyl, etc.; with proviso; X = CO or SO2; Y = absent or (un) substituted alkyl; and pharmaceutically acceptable salts, prodrugs and solvates thereof] were prepared as cannabinoid 1 (CB1) receptor modulators. For example, reaction of 2-methyl-1,5-diphenyl-1H-pyrrole-3-carboxylic acid with aniline gave 2-methyl-N,1,5-triphenyl-1H-pyrrole-3-carboxamide in 52% yield. I are active at the CB1 receptor (IC50 <1 micromolar), most preferred compds. have IC50 <200 nanomolar. Thus, I and their pharmaceutical compns. are useful for the treatment of obesity, psychiatric and neurol. disorders (no data).

ACCESSION NUMBER:

2004:565082 HCAPLUS

DOCUMENT NUMBER:

141:123553

TITLE:

Preparation of 1,5-diaryl-pyrrole-3-carboxamide derivatives as cannabinoid receptor modulators

INVENTOR (S):

Berggren, Anna Ingrid Kristina; Bostrom, Stig Jonas; Cheng, Leifeng; Elebring, Stig Thomas; Greasley,

Peter; Nagard, Mats; Wilstermann, Johan Michael;

Terricabras, Emma

PATENT ASSIGNEE(S):

Astrazeneca Ab, Swed.; Astrazeneca Uk Limited

SOURCE:

PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

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PATENT NO.
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PRIORITY APPLN. INFO.:
                                            GB 2002-30088
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OTHER SOURCE(S):
                        MARPAT 141:123553
     723303-38-6P 723303-39-7P 723303-40-0P
     723303-41-1P 723303-42-2P 723303-43-3P
     723303-44-4P 723303-45-5P 723303-46-6P
     723303-47-7P 723303-49-9P 723303-51-3P
     723303-53-5P 723303-55-7P 723303-57-9P
     723303-60-4P 723303-62-6P
    RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of 1,5-diaryl-pyrrole-3-carboxamide derivs. as CB1 modulators)
RN
     723303-38-6 HCAPLUS
     1H-Pyrrole-3-carboxamide, 2-methyl-N,1,5-triphenyl- (9CI) (CA INDEX NAME)
CN
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RN 723303-39-7 HCAPLUS CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-2-methyl-N,5-diphenyl- (9CI)

Young, Shawquia, Page 40

(CA INDEX NAME)

RN 723303-40-0 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-methoxyphenyl)-2-methyl-N,5-diphenyl- (9CI) (CA INDEX NAME)

RN 723303-41-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dichlorophenyl)-2-methyl-N,1-diphenyl-(9CI) (CA INDEX NAME)

RN 723303-42-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-5-(2,4-dichlorophenyl)-2-methyl-N-phenyl- (9CI) (CA INDEX NAME)

Young, Shawquia, Page 41

RN 723303-43-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dichlorophenyl)-1-(4-methoxyphenyl)-2-methyl-N-phenyl- (9CI) (CA INDEX NAME)

RN 723303-44-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dimethoxyphenyl)-2-methyl-N,1-diphenyl-(9CI) (CA INDEX NAME)

RN 723303-45-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-5-(2,4-dimethoxyphenyl)-2-methyl-N-phenyl- (9CI) (CA INDEX NAME)

RN 723303-46-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dimethoxyphenyl)-1-(4-methoxyphenyl)-2-methyl-N-phenyl- (9CI) (CA INDEX NAME)

RN 723303-47-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-methyl-1,5-diphenyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-49-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-2-methyl-5-phenyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-51-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-methoxyphenyl)-2-methyl-5-phenyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-53-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dichlorophenyl)-2-methyl-1-phenyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-55-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-5-(2,4-dichlorophenyl)-2-methyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-57-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dichlorophenyl)-1-(4-methoxyphenyl)-2-methyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-60-4 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-5-(2,4-dimethoxyphenyl)-2methyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

RN 723303-62-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(2,4-dimethoxyphenyl)-1-(4-methoxyphenyl)-2methyl-N-1-piperidinyl- (9CI) (CA INDEX NAME)

L4 ANSWER 12 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 11 Apr 2003

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. QLYR1[Q = I, C(:NH)NH2; R1 = (un)substituted alkyl, alkenyl, cycloalkyl, etc.; L = II-IV (wherein R4 = H, alkyl; R5 = H, alkyl, alkyl substituted by a substituted carbocyclic aryl), etc.; Y = SO2, CO, (CH2)m; m = 0-1] which act as MCH receptor antagonists, and are useful for prophylaxis or treatment of obesity, obesity related disorders, anxiety, or depression, were prepared Thus, hydrogenation of benzyl cis-[4-(4-dimethylaminoquinazolin-2-ylamino)cyclohexylmethyl]carbamate followed by reacting the resulting intermediate with 4-bromo-2-trifluoromethoxybenzaldehyde in the presence of NaBH(OAc)3 and AcOH in CH2Cl2, and treatment of the product with 4N HCl in EtOAc afforded 34% cis-V.2HCl which showed IC50 of 6 nM against MCH receptor.

ACCESSION NUMBER: 2003:282325 HCAPLUS

DOCUMENT NUMBER: 138:321285

TITLE: Preparation of quinazoline-2,4-diamines as MCH

receptor antagonists

INVENTOR(S): Sekiguchi, Yoshinori; Kanuma, Kosuke; Omodera,

Katsunori; Tran, Thuy-anh; Kramer, Bryan Aubrey;

Beeley, Nigel Robert Arnold

PATENT ASSIGNEE(S): Taisho Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 1171 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

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PRIORITY APPLN. INFO.:
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OTHER SOURCE(S):
                         MARPAT 138:321285
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     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of quinazoline-2,4-diamines as MCH receptor antagonists)
RN
     509143-54-8 HCAPLUS
CN
     1H-Pyrrole-3-carboxamide, N-[cis-4-[[4-(dimethylamino)-2-
     quinazolinyl]amino]cyclohexyl]-2-methyl-1,5-diphenyl- (9CI)
                                                                   (CA INDEX
     NAME)
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Relative stereochemistry.

Relative stereochemistry.

L4 ANSWER 13 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN ED Entered STN: 04 Apr 2003 GI

AB This invention relates to pyrrolecarboxamides and pyrrolecarbohydrazides (shown as I; variables defined below; e.g. 1-(2-chlorophenyl)-5-(4chlorophenyl) -2-methyl-N-(1-piperidinyl) -1H-pyrrole-3-carboxamide hydrochloride) that suppress appetite and induce weight loss. The invention also provides methods for synthesis of the compds., pharmaceutical compns. comprising the compds., and methods of using such compns. for inducing weight loss and treating obesity and obesity-related disorders. Although the methods of preparation are not claimed, 6 example prepns. of I and/or intermediates and characterization data for .apprx.50 examples of I are included. Seven pharmaceutical formulations are listed. Compds. of this invention are active in a fasted-refed acute feeding assay. For example, when 1-(2-chlorophenyl)-5-(4-chlorophenyl)-2-methyl-N-(1-piperidinyl)-1Hpyrrole-3-carboxamide hydrochloride was dosed at 10 mg/kg p.o., food consumption was reduced (relative to the food consumption observed for the vehicle control group) by up to 25% when measured at time points = 30-240 min. Likewise, when 1-(2-chlorophenyl)-5-(4-methoxyphenyl)-2,4-dimethyl-N'-[4-(trifluoromethyl)phenyl]-1H-pyrrole-3-carbohydrazide hydrochloride was dosed at 10 mg/kg p.o., food consumption was reduced by up to 35%. For I: R1 and R2 = Ph optionally substituted with ≥1 halogen, (C1-C6) alkyl, (C1-C6) alkoxy, trifluoromethyl, hydroxy, cyano, or nitro; R3 = H; R4 = CH3; R5 = H or (C1-C6)alkyl; R6 = substituted cyclohexyl; (un) substituted (C1-C5) alkyl; cyclopentyl, cycloheptyl or cyclo(C3-C7)alkyl-(C1-C3)alkyl, each of which may be optionally substituted; substituted benzyl; substituted phenyl; piperidin-4-yl, piperidin-3-yl, or pyrrolidin-3-yl, each of which may be optionally substituted on the N atom of the piperidine or pyrrolidine ring; -NR7R8. Or R5 and R6, taken together with the N atom to which they are attached, form a 5- to 10-membered saturated heterocyclic radical containing at least one addnl. N atom, with optional substitution. Or R5 and R6, taken together with the N atom to which they are attached, form a 1-piperidinyl, 1-pyrrolidinyl, or 1-morpholino group, which is substituted; addnl. details are given in the claims.

ACCESSION NUMBER: 2003:261810 HCAPLUS

DOCUMENT NUMBER: 138:287520 TITLE: Preparation

Preparation and use of pyrrolecarboxamides and pyrrolecarbohydrazides for treating obesity

INVENTOR(S): Smith, Roger A.; Kluender, Harold C. E.; Su, Ning;

Lavoie, Rico C.; Fan, Jianmei

PATENT ASSIGNEE(S):

Bayer Pharmaceuticals Corporation, USA

SOURCE: PCT Int. Appl., 62 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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APPLICATION NO.
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            CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
    CA 2461144
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                              . 20030403
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                                                                  20040305
PRIORITY APPLN. INFO.:
                                           US 2001-324441P
                                                                  20010924
                                           WO 2002-US30543
                                                                 20020924
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OTHER SOURCE(S): MARPAT 138:287520

IT 504405-88-3P, 2-Amino-1-(2-chlorophenyl)-5-(4-chlorophenyl)-N-cyclohexyl-1H-pyrrole-3-carboxamide

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation and use of pyrrolecarboxamides for treating obesity)

RN 504405-88-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-amino-1-(2-chlorophenyl)-5-(4-chlorophenyl)-N-cyclohexyl- (9CI) (CA INDEX NAME)

IT118179-43-4P, N-Cyclohexyl-1-(2,4-dichlorophenyl)-5-(4chlorophenyl) -2-methyl-1H-pyrrole-3-carboxamide 504405-37-2P, N-Cyclohexyl-2-methyl-1,5-diphenyl-1H-pyrrole-3-carboxamide 504405-38-3P, N-(4-Methylcyclohexyl)-2-methyl-1,5-diphenyl-1Hpyrrole-3-carboxamide 504405-39-4P, N-(Cyclohexylmethyl)-2methyl-1,5-diphenyl-1H-pyrrole-3-carboxamide 504405-40-7P, 1-(2-Chlorophenyl)-5-(4-methoxyphenyl)-2-methyl-N-(1-piperidinyl)-1Hpyrrole-3-carboxamide hydrochloride 504405-42-9P, N-Cyclohexyl-1-(2-chlorophenyl)-5-(4-methoxyphenyl)-2-methyl-1H-pyrrole-3carboxamide 504405-44-1P, 1-(2-Chlorophenyl)-5-(4-methoxyphenyl)-2-methyl-N'-[2-(trifluoromethyl)phenyl]-1H-pyrrole-3-carbohydrazide hydrochloride 504405-45-2P, N'-(3-(Trifluoromethyl)phenyl)-1-(2chlorophenyl) -5-(4-methoxyphenyl) -2-methyl-1H-pyrrole-3-carbohydrazide hydrochloride 504405-46-3P, N'-(4-(Trifluoromethyl)phenyl)-1-(2chlorophenyl) -5-(4-methoxyphenyl) -2-methyl-1H-pyrrole-3-carbohydrazide hydrochloride 504405-52-1P, N-(trans-2-(Benzyloxy)cyclohexyl)-1-(2,4-dichlorophenyl)-5-(4-chlorophenyl)-2-methyl-1H-pyrrole-3-carboxamide 504405-53-2P, N-(Piperidino)-1-(2,4-dichlorophenyl)-5-(4chlorophenyl)-2-methyl-1H-pyrrole-3-carboxamide hydrochloride 504405-54-3P, N'-(2-(Trifluoromethyl)phenyl)-1-(2,4dichlorophenyl) -5-(4-chlorophenyl) -2-methyl-1H-pyrrole-3-carbohydrazide hydrochloride 504405-55-4P, N'-(4-(Trifluoromethyl)phenyl)-1-(2,4-dichlorophenyl)-5-(4-chlorophenyl)-2-methyl-1H-pyrrole-3carbohydrazide hydrochloride 504405-56-5P, N-(trans-2-Hydroxycyclohexyl) -1-(2,4-dichlorophenyl) -5-(4-chlorophenyl) -2-methyl-1Hpyrrole-3-carboxamide 504405-57-6P, 5-(4-Chlorophenyl)-1-(2;4dichlorophenyl)-N-(cis-2-hydroxycyclohexyl)-2-methyl-1H-pyrrole-3carboxamide 504405-58-7P, N-(trans-2-(Benzyloxy)cyclohexyl)-1-(2chlorophenyl)-5-(4-chlorophenyl)-2-methyl-1H-pyrrole-3-carboxamide 504405-59-8P, 1-(2-Chlorophenyl)-5-(4-chlorophenyl)-2-methyl-N-(1piperidinyl)-1H-pyrrole-3-carboxamide hydrochloride 504405-61-2P , N-Cyclohexyl-1-(2-chlorophenyl)-5-(4-chlorophenyl)-2-methyl-1H-pyrrole-3carboxamide 504405-62-3P, 1-(2-Chlorophenyl)-5-(4-chlorophenyl)-2-methyl-N'-[2-(trifluoromethyl)phenyl]-1H-pyrrole-3-carbohydrazide hydrochloride 504405-64-5P, N'-(4-(Trifluoromethyl)phenyl)-1-(2chlorophenyl)-5-(4-chlorophenyl)-2-methyl-1H-pyrrole-3-carbohydrazide hydrochloride 504405-65-6P, 1-(2-Chlorophenyl)-5-(4chlorophenyl) -N-(trans-2-hydroxycyclohexyl) -2-methyl-1H-pyrrole-3carboxamide 504405-66-7P, N-(cis-2-Hydroxycyclohexyl)-1-(2chlorophenyl) -5-(4-chlorophenyl) -2-methyl-1H-pyrrole-3-carboxamide 504405-67-8P, N-((4-Chlorophenyl)methyl)-1-(2,4-dichlorophenyl)-5-

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(4-chlorophenyl)-2-methyl-1H-pyrrole-3-carboxamide 504405-68-9P,
N-((4-Fluorophenyl)methyl)-1-(2,4-dichlorophenyl)-5-(4-chlorophenyl)-2-
methyl-1H-pyrrole-3-carboxamide 504405-69-0P,
N-((4-(Trifluoromethyl)phenyl)methyl)-1-(2,4-dichlorophenyl)-5-(4-
chlorophenyl) -2-methyl-1H-pyrrole-3-carboxamide 504405-70-3P,
N-(4-Fluorophenyl)-1-(2,4-dichlorophenyl)-5-(4-chlorophenyl)-2-methyl-1H-
pyrrole-3-carboxamide 504405-71-4P, N-(1-Benzylpiperidin-4-yl)-1-
(2,4-dichlorophenyl)-5-(4-chlorophenyl)-2-methyl-1H-pyrrole-3-carboxamide
504405-80-5P, N-Cyclohexyl-1-(2-chlorophenyl)-5-(4-methoxyphenyl)-
2,4-dimethyl-1H-pyrrole-3-carboxamide 504405-81-6P,
1-(2-Chlorophenyl)-5-(4-methoxyphenyl)-2,4-dimethyl-N'-[4-
(trifluoromethyl)phenyl]-1H-pyrrole-3-carbohydrazide hydrochloride
504405-82-7P, 2-Amino-1-(2-chlorophenyl)-5-(4-chlorophenyl)-N-
cyclohexyl-1H-pyrrole-3-carboxamide hydrochloride 504405-83-8P,
2-Amino-1-phenyl-5-(4-chlorophenyl)-N-cyclohexyl-1H-pyrrole-3-carboxamide
hydrochloride 504405-84-9P, 2-Amino-1-(2-fluorophenyl)-5-(4-
chlorophenyl)-N-cyclohexyl-1H-pyrrole-3-carboxamide hydrochloride
504405-85-0P, 2-Amino-1-(2-bromophenyl)-5-(4-chlorophenyl)-N-
cyclohexyl-1H-pyrrole-3-carboxamide hydrochloride 504405-86-1P,
2-Amino-1-(2,4-dichlorophenyl)-5-(4-chlorophenyl)-N-cyclohexyl-1H-pyrrole-
3-carboxamide hydrochloride
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)
   (drug candidate; preparation and use of pyrrolecarboxamides for treating
   obesity-related disorders)
118179-43-4 HCAPLUS
1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-N-cyclohexyl-1-(2,4-
dichlorophenyl) - 2-methyl- (9CI) (CA INDEX NAME)
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RN

CN

RN 504405-38-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-methyl-N-(4-methylcyclohexyl)-1,5-diphenyl-(9CI) (CA INDEX NAME)

RN 504405-39-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-(cyclohexylmethyl)-2-methyl-1,5-diphenyl-(9CI) (CA INDEX NAME)

RN 504405-40-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2-chlorophenyl)-5-(4-methoxyphenyl)-2-methyl-N-1-piperidinyl-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 504405-42-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2-chlorophenyl)-N-cyclohexyl-5-(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)

RN 504405-44-1 HCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 1-(2-chlorophenyl)-5-(4-methoxyphenyl)-2-methyl-, 2-[2-(trifluoromethyl)phenyl]hydrazide, hydrochloride (9CI) (CA INDEX NAME)

RN 504405-45-2 HCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 1-(2-chlorophenyl)-5-(4-methoxyphenyl)-2-methyl-, 2-[3-(trifluoromethyl)phenyl]hydrazide, hydrochloride (9CI) (CA INDEX NAME)

RN 504405-46-3 HCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 1-(2-chlorophenyl)-5-(4-methoxyphenyl)-2-methyl-, 2-[4-(trifluoromethyl)phenyl]hydrazide, hydrochloride (9CI) (CA INDEX NAME)

RN 504405-52-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-2-methyl-N-[(1R,2R)-2-(phenylmethoxy)cyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 504405-53-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-2-methyl-N-1-piperidinyl-, hydrochloride (9CI) (CA INDEX NAME)

RN 504405-54-3 HCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-2-methyl-, 2-[2-(trifluoromethyl)phenyl]hydrazide, hydrochloride (9CI) (CA INDEX NAME)

RN 504405-55-4 HCAPLUS
CN 1H-Pyrrole-3-carboxylic acid, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-2methyl-, 2-[4-(trifluoromethyl)phenyl]hydrazide, hydrochloride (9CI) (CA
INDEX NAME)

RN 504405-56-5 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-N[(1R,2R)-2-hydroxycyclohexyl]-2-methyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 504405-57-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-N[(1R,2S)-2-hydroxycyclohexyl]-2-methyl-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 504405-58-7 HCAPLUS

CN lH-Pyrrole-3-carboxamide, 1-(2-chlorophenyl)-5-(4-chlorophenyl)-2-methyl-N[(1R,2R)-2-(phenylmethoxy)cyclohexyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 504405-59-8 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2-chlorophenyl)-5-(4-chlorophenyl)-2-methyl-N-1-piperidinyl-, hydrochloride (9CI) (CA INDEX NAME)

•x HCl

RN 504405-61-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2-chlorophenyl)-5-(4-chlorophenyl)-N-cyclohexyl-2-methyl- (9CI) (CA INDEX NAME)

RN 504405-62-3 HCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 1-(2-chlorophenyl)-5-(4-chlorophenyl)-2-methyl-, 2-[2-(trifluoromethyl)phenyl]hydrazide, hydrochloride (9CI) (CA INDEX NAME)

RN 504405-64-5 HCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 1-(2-chlorophenyl)-5-(4-chlorophenyl)-2-methyl-, 2-[4-(trifluoromethyl)phenyl]hydrazide, hydrochloride (9CI) (CA INDEX NAME)

RN 504405-65-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2-chlorophenyl)-5-(4-chlorophenyl)-N-[(1R,2R)-2-hydroxycyclohexyl]-2-methyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 504405-66-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2-chlorophenyl)-5-(4-chlorophenyl)-N-[(1R,2S)-2-hydroxycyclohexyl]-2-methyl-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 504405-67-8 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-N-[(4-chlorophenyl)methyl]-1-(2,4-dichlorophenyl)-2-methyl-(9CI) (CA INDEX NAME)

RN 504405-68-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-N-[(4-fluorophenyl)methyl]-2-methyl- (9CI) (CA INDEX NAME)

RN 504405-69-0 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-2methyl-N-[[4-(trifluoromethyl)phenyl]methyl]- (9CI) (CA INDEX NAME)

RN 504405-70-3 HCAPLUS CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-N-(4-fluorophenyl)-2-methyl- (9CI) (CA INDEX NAME)

RN 504405-71-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-2-methyl-N-[1-(phenylmethyl)-4-piperidinyl]- (9CI) (CA INDEX NAME)

RN 504405-80-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2-chlorophenyl)-N-cyclohexyl-5-(4-methoxyphenyl)-2,4-dimethyl- (9CI) (CA INDEX NAME)

RN 504405-81-6 HCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 1-(2-chlorophenyl)-5-(4-methoxyphenyl)-2,4-dimethyl-, 2-[4-(trifluoromethyl)phenyl]hydrazide, hydrochloride (9CI) (CA INDEX NAME)

RN 504405-82-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-amino-1-(2-chlorophenyl)-5-(4-chlorophenyl)-N-cyclohexyl-, hydrochloride (9CI) (CA INDEX NAME)

•x HCl

RN 504405-83-8 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-amino-5-(4-chlorophenyl)-N-cyclohexyl-1-phenyl-, hydrochloride (9CI) (CA INDEX NAME)

•x HCl

RN 504405-84-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-amino-5-(4-chlorophenyl)-N-cyclohexyl-1-(2-fluorophenyl)-, hydrochloride (9CI) (CA INDEX NAME)

•x HCl

RN 504405-85-0 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-amino-1-(2-bromophenyl)-5-(4-chlorophenyl)-N-cyclohexyl-, hydrochloride (9CI) (CA INDEX NAME)

•x HCl

RN 504405-86-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-amino-5-(4-chlorophenyl)-N-cyclohexyl-1-(2,4-dichlorophenyl)-, hydrochloride (9CI) (CA INDEX NAME)

REFERENCE COUNT:

THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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ED Entered STN: 15 Nov 2002

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The title compds. [I; Ar = (un)substituted Ph, pyridyl, thienyl, etc.; A = (un)substituted Ph, thienyl, furanyl, etc.; Y = 0, NH, CONHCH2, SOn, CH2, a bond; R2 = H, halo, CF3, CN, alkyl; R1, R3, R4 = H, alkyl, CH2Ph; X = 0, S, CH2; n = 0-2], useful as antagonists of urotensin II, were prepared and formulated. E.g., a 6-step synthesis of (R)-II, starting from 2-chloro-5-nitroanisole, was given. Activity for the compds. I against h-U-II range from Ki = 10-10000 nM.

ACCESSION NUMBER:

2002:868728 HCAPLUS

DOCUMENT NUMBER:

137:370085

TITLE:

Preparation of sulfonamides as antagonists of

urotensin II

INVENTOR(S): Dhanak, Dashyant; Gallagher, Timothy F.; Knight,

Steven D.

PATENT ASSIGNEE(S): Smithkline Beecham Corporation, USA

SOURCE: PCT Int. Appl., 26 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.					KIND DATE			APPLICATION NO.					DATE				
	WO 2002089793				A1	-	20021114		WO 2002-US14409					20020507				
		W:						AU,										
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,
			LS,	LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	OM,	PH,
			PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TN,	TR,	TT,	TZ,
			UA,	UG,	US,	UΖ,	VN,	YU,	ZA,	ZM,	ZW,	AM,	ΑZ,	BY,	KG,	KZ,	MD,	RU,
			ТJ,	TM														
		RW:	GH,	GM,	KΕ,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑT,	BE,	CH,
			CY,	DE,	DK,	ES,	FI,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,
			BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
	EP 1387679				A1 20040211				EP 2002-769373					20020507				
		R:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙT,	LI,	LU,	NL,	SE,	MC,	PT,
								RO,										
	JP 2004529164					T2 20040924				JP 2002-586928				20020507				
US 2004198979					A1 20041007				US 2003-477051				20031107					
PRIORITY APPLN. INFO.:					. :					1	US 2	001-	2893	05P]	P 2	0010	507
										1	US 2	001-2	2893	07P]	P 2	0010	507
										1	WO 2	002-1	JS144	109	1	W 2	0020	507
OTHER SOURCE(S):						MARI	РАТ	137.	37009	35								

OTHER SOURCE(S): MARPAT 137:370085

IT 474947-42-7P 474947-44-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of sulfonamides as antagonists of urotensin II)

RN 474947-42-7 HCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 4-[[[4-chloro-3-[[(3R)-1-methyl-3-pyrrolidinyl]oxy]phenyl]amino]sulfonyl]-2-(4-chlorophenyl)-5-methyl-1-phenyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 474947-44-9 HCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 4-[[[4-chloro-3-[[(3R)-1-methyl-3-pyrrolidinyl]oxy]phenyl]amino]sulfonyl]-5-methyl-1,2-diphenyl-, ethyl

(CA INDEX NAME) ester (9CI)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4ANSWER 15 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

2

ED Entered STN: 01 Jul 1999

AΒ The calcn. of possible mol. formulas on the basis of the very precise ESI-FT-ICR measurement thus gave solely the correct composition This rapid mol. formula determination may also be applied to complex mixts. such as those which arise from combinatorial chemical To demonstrate the performance of this method in this respect, a split-mix compound collection of 140 different pyrrole amides consisting of 10 subcollections of 14 compds. each was synthesized on Rink amide AM resin. The results of the subcollection with 2-bromoacetophenone as building block (R2=C6H5, R3=H) are illustrated as an example. The total amount of sample of 20 pmol gives a mean sample consumption of 1.4 pmol per compound for the routine measurement. All 14 expected products could be detected by mass spectrometry.

ACCESSION NUMBER: 1999:404464 HCAPLUS

DOCUMENT NUMBER: 131:193473

TITLE: ESI Fourier transform ion cyclotron resonance mass

> spectrometry (ESI-FT-ICR-MS): a rapid high-resolution analytical method for combinatorial compound libraries

Walk, Tilmann B.; Trautwein, Axel W.; Richter, AUTHOR (S):

Hartmut; Jung, Gunther

Institut fur Organische Chemie der Universitat, CORPORATE SOURCE:

Tubingen, D-72076, Germany

SOURCE: Angewandte Chemie, International Edition (1999),

38(12), 1763-1765

CODEN: ACIEF5; ISSN: 1433-7851

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

239474-84-1 239474-93-2 239474-97-6

RL: ANT (Analyte); PEP (Physical, engineering or chemical process); ANST (Analytical study); PROC (Process)

(ESI Fourier transform ion cyclotron resonance mass spectrometry for

rapid high-resolution anal. of combinatorial compds. of)

RN239474-84-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-cyclopropyl-2-methyl-5-phenyl- (9CI) (CA INDEX NAME)

Me
$$\stackrel{N}{\longrightarrow}$$
 Ph

RN 239474-93-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,3-dihydro-1H-inden-1-yl)-2-methyl-5-phenyl-(9CI) (CA INDEX NAME)

$$\stackrel{\text{Ph}}{\underset{\text{O}}{\bigvee}}$$

RN 239474-97-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-methyl-5-phenyl-1-[1-(phenylmethyl)-4-piperidinyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Ph} & \text{CH}_2\text{--Ph} \\ & & \\ \text{H}_2\text{N}\text{--C} & \text{Me} \\ & & \\ \text{O} & \end{array}$$

REFERENCE COUNT:

19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 28 Feb 1996

AB A number of new title compds. (6) have been synthesized by the reaction of N-methyl/N,N-diethylacetoacetamide with benzoin and various alkyl, aryl and aralkylamines in the presence of formic acid. Compds. 6 showed appreciable antifungal activity mild bactericidal activity.

ACCESSION NUMBER:

1996:122149 HCAPLUS

DOCUMENT NUMBER:

124:289156

TITLE:

Synthesis of some new 4,5-diphenyl-3-(N-methyl/N,N-diethyl)carbamoyl-2-methyl-1-substituted-1H-pyrroles

and their fungicidal activity

AUTHOR (S):

Sadanandam, Y. S.; Leelavathi, P.; Shetty, Meera M.

Young, Shawquia, Page 72

CORPORATE SOURCE:

Organic Chemistry Division-I, Indian Institute

Chemical Technology, Hyderabad, 500 007, India

SOURCE:

Indian Journal of Heterocyclic Chemistry (1995), 5(2),

125-8

CODEN: IJCHEI; ISSN: 0971-1627

PUBLISHER:

Lucknow University, Dep. of Chemistry

DOCUMENT TYPE:

Journal

LANGUAGE:

English

175475-93-1P 175475-94-2P 175475-95-3P IT

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); BIOL (Biological

study); PREP (Preparation)

(preparation and antimicrobial activity of)

RN 175475-93-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N,2-dimethyl-1,4,5-triphenyl- (9CI) (CA INDEX

NAME)

RN175475-94-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N,2-dimethyl-1-(4-methylphenyl)-4,5-diphenyl-

(9CI) (CA INDEX NAME)

RN 175475-95-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N,2-dimethyl-4,5-diphenyl-(CA INDEX NAME)

IT 175475-96-4P 175475-97-5P 175475-98-6P

175475-99-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 175475-96-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-methoxyphenyl)-N,2-dimethyl-4,5-diphenyl-(9CI) (CA INDEX NAME)

RN 175475-97-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N,2-dimethyl-1-(2-nitrophenyl)-4,5-diphenyl-(9CI) (CA INDEX NAME)

RN 175475-98-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N,2-dimethyl-1-(4-nitrophenyl)-4,5-diphenyl-(9CI) (CA INDEX NAME)

RN 175475-99-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(3,4-dichlorophenyl)-N,2-dimethyl-4,5-diphenyl-(9CI) (CA INDEX NAME)

L4 ANSWER 17 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 15 Feb 1996

AB Several fused pyrimidinones were synthesized by reaction of aminoarenecarboxamide with esters in moderate to good yields. In the presence of sodium ethoxide, treatments of 2-amino-1-phenyl-3-pyrrolecarboxamide, 2-amino-3-thiophenecarboxamide, 3-amino-4-isoxazolecarboxamide, 4-amino-1,2,3-triazole-5-carboxamide, and o-aminobenzamide with esters such as Et formate and Et acetate led to the corresponding pyrrolo[2,3-d]- and thieno[2,3-d]pyrimidin-4(3H)-ones, isoxazolo[5,4-d]pyrimidin-4(5H)-ones, 1,2,3-triazolo[4,5-d]pyrimidin-7(6H)-ones, and -4(3H)-quinazolones, resp.

ACCESSION NUMBER:

1996:97030 HCAPLUS

DOCUMENT NUMBER:

124:260966

TITLE:

Synthesis of fused pyrimidinones by reaction of aminoarenecarboxamide with esters; preparation of pyrrolo[2,3-d]-, thieno[2,3-d]-, isoxazolo[5,4-d]-,

and 1,2,3-triazolo[4,5-d]pyrimidinones, and

-quinazolones

AUTHOR(S): Miyashita, Akira; Fujimoto, Katsuhiro; Okada, Tomomi;

Higashino, Takeo

CORPORATE SOURCE: Sch. Pharm. Sci., Univ. Shizuoka, Shizuoka, 422, Japan

SOURCE: Heterocycles (1996), 42(2), 691-9 CODEN: HTCYAM; ISSN: 0385-5414

PUBLISHER: Japan Institute of Heterocyclic Chemistry

DOCUMENT TYPE: Journal LANGUAGE: English

IT 56023-01-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(synthesis of fused pyrimidinones by reaction of aminoarenecarboxamide

with esters)

RN 56023-01-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-amino-1,4,5-triphenyl- (9CI) (CA INDEX NAME)

ANSWER 18 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Entered STN: 30 Mar 1993

ED GI

T.4

The synthesis and anti-Candida activity of some 3-aminomethyl-1,5-diaryl-2-methylpyrroles, e.g., I (R = H, 4-Cl, 4-F, 2,4-Cl2; R1 = H, Cl; R2 = NMe2, NHPh, pyrrolidino, 1-imidazolyl, 4-methylpiperazin-1-yl) are reported. Some derivs. show a rather strong anti-Candida activity. On the basis of exptl. results, microbiol. activity of 1,5-diarylpyrroles appears to be mainly related to aminic nitrogen lone pair availability of C3 substituent of the pyrrole nucleus. The C5 and N1 substituents play an important role in modulating biol. activity. Some structure-activity relationships are proposed.

ACCESSION NUMBER: 1993:124338 HCAPLUS

Ι

DOCUMENT NUMBER: 118:124338

TITLE: Studies on anti-Candida agents with a pyrrole moiety.

Synthesis and microbiological activity of some

3-(aminomethyl)-1,5-diaryl-2-methylpyrrole derivatives AUTHOR(S):

Cerreto, F.; Villa, A.; Retico, A.; Scalzo, M.

CORPORATE SOURCE: Dip. Studi Chim. Technol. Sostanze Biol. Attive, Univ.

La Sapienza, Rome, 00185, Italy European Journal of Medicinal Chemistry (1992), 27(7),

701-8

CODEN: EJMCA5; ISSN: 0223-5234

DOCUMENT TYPE:

Journal English

LANGUAGE:

SOURCE:

IT 146204-80-0P 146204-81-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); BIOL (Biological

study); PREP (Preparation)

(preparation and antifungal activity of)

RN146204-80-0 HCAPLUS

1H-Pyrrole-3-carboxamide, 1,5-bis(4-chlorophenyl)-2-methyl- (9CI) CNINDEX NAME)

$$\begin{array}{c} C1 \\ \\ Me \\ \\ N-C \\ \\ \\ O \end{array}$$

RN146204-81-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1,5-bis(4-chlorophenyl)-N,N,2-trimethyl- (9CI) (CA INDEX NAME)

$$Me_{2}N-C$$

$$0$$

$$C1$$

$$C1$$

$$C1$$

L4ANSWER 19 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 30 Mar 1993

AΒ The synthesis of some [(1-alkyl), (1-aryl) and (1-benzyl)-5-aryl-3-

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carboxamido-2-methyl]pyrrole derivs. is reported. Their activity against Candida strains was assessed and the structure-activity relationships for these compds. are discussed and related to structure-activity guidelines proposed for a series of previously studied 1,5-diarylpyrroles.

ACCESSION NUMBER: 1993:120801 HCAPLUS

DOCUMENT NUMBER: 118:120801

TITLE: Studies on anti-Candida agents with a pyrrole moiety.

Synthesis and microbiological activity of some [(1-alkyl),(1-aryl) and (1-benzyl)-5-aryl-3-

carboxamido-2-methyl]pyrrole derivatives

AUTHOR(S): Scalzo, Marcello; Biava, Mariangela; Cerreto, Felice;

Villa, Adelaide

CORPORATE SOURCE: Dip. Studi Chim. Tecnol., Univ. "La Sapienza", Rome,

Italy

SOURCE: Farmaco (1992), 47(7-8), 1047-53

CODEN: FRMCE8; ISSN: 0014-827X

DOCUMENT TYPE: Journal LANGUAGE: English

IT 146429-89-2P 146429-90-5P 146429-91-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); BIOL (Biological

study); PREP (Preparation)

(preparation and fungicidal activity of)

RN 146429-89-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2-chlorophenyl)-N,N-bis(2-hydroxyethyl)-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
C1 & NO_2 \\
Me & N \\
HO-CH_2-CH_2 & \\
HO-CH_2-CH_2-N-C & \\
O & O
\end{array}$$

RN 146429-90-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N,N-bis(2-hydroxyethyl)-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{Me} \\ \text{NO}_2 \\ \text{HO-} \text{CH}_2 - \text{CH}_2 - \text{NO}_2 \\ \text{O} \end{array}$$

RN 146429-91-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N,N-bis(2-hydroxyethyl)-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & & \\ \text{Me} & & & & \\ \text{HO}-\text{CH}_2-\text{CH}_2 & & & \\ \text{HO}-\text{CH}_2-\text{CH}_2-\text{N}-\text{C} & & \\ & & & & \\ & & & & \\ & & & & \\ \end{array}$$

L4 ANSWER 20 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 24 Jan 1992

AB The correlation between lipophilicity and activity against Candida

albicans of some 1,5-diarylpyrroles is described.

ACCESSION NUMBER:

1992:18272 HCAPLUS

DOCUMENT NUMBER:

116:18272

TITLE:

Correlation analysis in a set of 1,5-diarylpyrroles

with antimycotic activity

AUTHOR (S):

Scalzo, M.; Biava, M.; Porretta, G. C.; Cerreto, F.

Fac. Farm., Univ. "La Sapienza", Rome, Italy

CORPORATE SOURCE: SOURCE:

Pharmacochemistry Library (1991), 16 (QSAR: Ration.

Approaches Des. Bioact. Compd.), 389-92

CODEN: PHLIDQ; ISSN: 0165-7208

DOCUMENT TYPE:

Journal English

LANGUAGE: E
IT 138147-74-7D, derivs.

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(antimycotic activity of, QSAR of)

RN 138147-74-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-methyl-1,5-diphenyl- (9CI) (CA INDEX NAME)

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Ph Me C-NH<sub>2</sub>
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ANSWER 21 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
L4
     Entered STN: 16 Sep 1989
ED
AB
     A series of 1,5-diarylpyrrole derivs. were synthesized and tested in vitro
     for their activity against bacteria and fungi. Forty-eight derivs. were
     evaluated for their antifungal activity against Candida albicans and
     various strains of Candida species. The antibacterial activity of 10
     derivs. was evaluated against gram-pos. and gram-neg. bacteria.
     Structure-activity relations are discussed.
ACCESSION NUMBER:
                         1989:493768 HCAPLUS
DOCUMENT NUMBER:
                         111:93768
TITLE:
                         Synthesis and microbiological activity of new
                         1,5-diarylpyrroles
AUTHOR (S):
                         Scalzo, Marcello; Biava, Mariangela; Cerreto, Felice;
                         Porretta, Giulo Cesare; Panico, Salvatore; Simonetti,
                         Fac. Farm., Univ. La Sapienza, Rome, Italy
CORPORATE SOURCE:
                         European Journal of Medicinal Chemistry (1988), 23(6),
SOURCE:
                         CODEN: EJMCA5; ISSN: 0223-5234
DOCUMENT TYPE:
                         Journal
LANGUAGE:
                         English
OTHER SOURCE(S):
                         CASREACT 111:93768
     122121-42-0P 122121-43-1P 122121-44-2P
     122121-45-3P 122121-47-5P 122121-48-6P
     122121-49-7P 122121-50-0P 122121-52-2P
     122121-53-3P 122121-54-4P 122121-55-5P
     122121-57-7P 122121-58-8P 122121-59-9P
     122121-60-2P 122121-62-4P 122121-63-5P
     122121-64-6P 122121-65-7P 122121-67-9P
     122121-68-0P 122121-69-1P 122121-70-4P
     122121-71-5P 122121-72-6P 122121-73-7P
     122148-64-5P
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); BIOL (Biological
     study); PREP (Preparation)
        (preparation and antimicrobial activity of)
RN
     122121-42-0 HCAPLUS
CN
     1H-Pyrrole-3-carboxamide, 1-(4-fluorophenyl)-N-hexyl-2-methyl-5-(4-
    nitrophenyl) - (9CI) (CA INDEX NAME)
```

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{CH}_2) \\ \text{5} \\ \text{NH} \\ \text{C} \\ \text{O} \end{array}$$

RN 122121-43-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-dodecyl-1-(4-fluorophenyl)-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 122121-44-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-fluorophenyl)-2-methyl-5-(4-nitrophenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

RN 122121-45-3 HCAPLUS

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CN 1H-Pyrrole-3-carboxamide, N-[(4-chlorophenyl)methyl]-1-(4-fluorophenyl)-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 122121-47-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-bromophenyl)-N-hexyl-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 122121-48-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-bromophenyl)-N-dodecyl-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Me
$$\sim$$
 NO2

Me (CH₂)₁₁-NH-C

NO2

RN 122121-49-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-bromophenyl)-2-methyl-5-(4-nitrophenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Br} \\ \text{Me} \\ \text{NO}_2 \\ \text{Ph-CH}_2-\text{NH-C} \\ \text{O} \\ \end{array}$$

RN 122121-50-0 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-bromophenyl)-N-[(4-chlorophenyl)methyl]-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 122121-52-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-hexyl-2-methyl-5-(4-nitrophenyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

$$F_3C$$
 NO_2
 $Me-(CH_2)_5-NH-C$
 O

RN 122121-53-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-dodecyl-2-methyl-5-(4-nitrophenyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} F_3C \\ \hline \\ Me - (CH_2)_{11} - NH - C \\ \hline \\ O \end{array}$$

RN 122121-54-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-methyl-5-(4-nitrophenyl)-N-(phenylmethyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} F_3C \\ \hline \\ NO_2 \\ \hline \\ Ph-CH_2-NH-C \\ \hline \\ O \\ \end{array}$$

RN 122121-55-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[(4-chlorophenyl)methyl]-2-methyl-5-(4-nitrophenyl)-1-[3-(trifluoromethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 122121-57-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-[2-chloro-5-(trifluoromethyl)phenyl]-N-hexyl-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{CF}_3 \\ & \text{Me} & \text{NO}_2 \\ & \text{Me} - (\text{CH}_2)_5 - \text{NH} - \text{C} \\ & \text{II} \\ & \text{O} \end{array}$$

RN 122121-58-8 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-[2-chloro-5-(trifluoromethyl)phenyl]-N-dodecyl-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

$$C1$$
 Me
 NO_2
 Me
 CF_3
 Me
 NO_2
 Me
 O

RN 122121-59-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-[2-chloro-5-(trifluoromethyl)phenyl]-2-methyl-5-(4-nitrophenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} \text{CF}_3 \\ \text{Me} & \text{NO}_2 \\ \text{Ph-CH}_2-\text{NH-C} \\ \text{O} \end{array}$$

RN 122121-60-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[(4-chlorophenyl)methyl]-1-[2-chloro-5-(trifluoromethyl)phenyl]-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 122121-62-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(3,5-dichlorophenyl)-N-hexyl-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Cl} & \text{Cl} \\ & \text{Me} & \text{NO}_2 \\ & \text{Me} - (\text{CH}_2)_5 - \text{NH} - \text{C} \\ & \text{O} \end{array}$$

RN 122121-63-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(3,5-dichlorophenyl)-N-dodecyl-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Cl} & \text{Cl} \\ \text{Me} & \text{NO}_2 \\ \text{Me} - (\text{CH}_2)_{11} - \text{NH} - \text{C} \\ \parallel & \text{O} \end{array}$$

RN 122121-64-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(3,5-dichlorophenyl)-2-methyl-5-(4-nitrophenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Cl} & \text{Cl} \\ & \text{Me} & \text{NO}_2 \\ & \text{Ph-CH}_2-\text{NH-C} \\ & \text{O} \end{array}$$

RN 122121-65-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[(4-chlorophenyl)methyl]-1-(3,5-dichlorophenyl)-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 122121-67-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(3,4-dichlorophenyl)-N-hexyl-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Me (CH₂)₅ - NH - C
$$\begin{vmatrix} & & & & & & & & \\ & & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\ & & \\ & \\ & & \\ & \\ & & \\ & \\ & & \\ & & \\ & \\ & & \\ & \\ &$$

RN 122121-68-0 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(3,4-dichlorophenyl)-N-dodecyl-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} & \\ & \text{C1} & \\ & \text{Me} & \\ & \text{Me} & \\ & \text{Me} & \\ & \text{CH}_2)_{11} - \text{NH} - \\ & \text{C} & \\ & \text{O} & \\ \end{array}$$

RN 122121-69-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(3,4-dichlorophenyl)-2-methyl-5-(4-nitrophenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Cl} & \\ & \text{NO}_2 \\ & \text{NP} - \text{CH}_2 - \text{NH} - \text{C} \\ & \text{O} \end{array}$$

RN 122121-70-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-[(4-chlorophenyl)methyl]-1-(3,4-dichlorophenyl)-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 122121-71-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-dodecyl-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} \\ & \text{NO}_2 \\ \text{Me} & \text{N} \\ & \text{NO}_2 \\ \text{Me} & \text{CH}_2)_{11} - \text{NH} - \text{C} \\ & \text{O} \\ \end{array}$$

RN 122121-72-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-2-methyl-5-(4-nitrophenyl)-N-(phenylmethyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} \\ & \\ \text{NO}_2 \\ \text{Me} & \\ & \\ \text{N} \\ & \\ \text{NO}_2 \\ \\ & \\ \text{Ph-CH}_2-\text{NH-C} \\ \\ & \\ & \\ \text{O} \\ \end{array}$$

RN 122121-73-7 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-[(4-chlorophenyl)methyl]-1-(2,4-dichlorophenyl)-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 122148-64-5 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-hexyl-2-methyl-5-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Cl} \\ \text{NO}_2 \\ \text{Me} - \text{(CH}_2)_5 - \text{NH} - \text{C} \\ \text{O} \end{array}$$

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ED. Entered STN: 04 Feb 1989

GI

$$\mathbb{R}^{2}$$

$$\mathbb{R}^{2}$$

$$\mathbb{R}^{n}$$

The synthesis and antifungal activities of new 1,5-diarylpyrrole derivs. I AΒ (R = NO2, Cl; R1 = HNC6H11, HNC12H25, HNC6H13, N-methylpiperazinyl; R2 = H, NO2; n = 1 or 2) are reported. In comparison with pyrrolnitrin, only carboxamide derivs. exhibit satisfactory antifungal activity. All the compds. show very poor antibacterial activity. The displacement of the ${\tt NO2}$ group from the para to the meta or ortho positions of the aryl at C5

of the pyrrole ring affects the antimicrobial activity. 110:36649

ACCESSION NUMBER: DOCUMENT NUMBER:

1989:36649 HCAPLUS

TITLE:

Compounds with antibacterial and antifungal activity. Part IV. Synthesis and microbiological activity of

new 1,5-diarylpyrrole derivatives

AUTHOR (S):

Scalzo, M.; Porretta, G. C.; Chimenti, F.; Casanova,

M. C.; Panico, S.; Simonetti, N.

CORPORATE SOURCE:

Dip. Chim. Tecnol. Sostanze Biol. Attive, Univ. "La

Sapienza", Rome, Italy

SOURCE:

Farmaco, Edizione Scientifica (1988), 43(9), 665-76

CODEN: FRPSAX; ISSN: 0430-0920

DOCUMENT TYPE: LANGUAGE:

Journal

Italian CASREACT 110:36649

OTHER SOURCE(S):

118209-76-0P 118209-77-1P 118209-78-2P

118209-80-6P 118209-81-7P 118209-82-8P

118209-83-9P 118209-84-0P 118209-85-1P 118209-87-3P 118209-88-4P 118209-89-5P 118209-91-9P 118209-92-0P 118209-93-1P 118209-94-2P 118209-95-3P 118209-97-5P 118209-98-6P 118209-99-7P 118210-01-8P 118210-02-9P 118210-03-0P 118210-05-2P 118210-06-3P 118210-07-4P 118228-53-8P RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation) (preparation and antimicrobial activity of) 118209-76-0 HCAPLUS RN CN 1H-Pyrrole-3-carboxamide, N-cyclohexyl-2-methyl-1-(4-nitrophenyl)-5-phenyl-(9CI) (CA INDEX NAME)

RN 118209-77-1 HCAPLUS CN 1H-Pyrrole-3-carboxamide, N-dodecyl-2-methyl-1-(4-nitrophenyl)-5-phenyl-(9CI) (CA INDEX NAME)

Me
$$\sim$$
 Ph Me (CH₂)₁₁-NH-C

RN 118209-78-2 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-hexyl-2-methyl-1-(4-nitrophenyl)-5-phenyl(9CI) (CA INDEX NAME)

Young, Shawquia, Page 95

Me
$$\sim$$
 NO₂

Me \sim NH Ph

Me (CH₂)₅ - NH - C

RN 118209-80-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-cyclohexyl-2-methyl-5-phenyl- (9CI) (CA INDEX NAME)

RN 118209-81-7 HCAPLUS CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-dodecyl-2-methyl-5-phenyl-(9CI) (CA INDEX NAME)

Me (CH₂)
$$_{11}$$
 - NH - C $_{0}$

RN 118209-82-8 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-hexyl-2-methyl-5-phenyl(9CI) (CA INDEX NAME)

Me
$$\sim$$
 \sim Ph

Me (CH₂)₅-NH-C

 \sim 0

RN 118209-83-9 HCAPLUS CN 1H-Pyrrole-3-carboxamide, N-cyclohexyl-1-(2,4-dichlorophenyl)-2-methyl-5phenyl- (9CI) (CA INDEX NAME)

RN 118209-84-0 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-dodecyl-2-methyl-5-phenyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Cl} \\ & \text{Me} & \text{N} \\ & \text{N} \end{array} \begin{array}{c} \text{Ph} \\ & \text{N} \\ & \text{O} \end{array}$$

RN 118209-85-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-hexyl-2-methyl-5-phenyl-(9CI) (CA INDEX NAME)

$$C1$$
 Me
 N
 Ph
 $Me^- (CH2)5-NH-C$
 0

RN 118209-87-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-cyclohexyl-2-methyl-5-(2-nitrophenyl)-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118209-88-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-dodecyl-2-methyl-5-(2-nitrophenyl)-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118209-89-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-hexyl-2-methyl-5-(2-nitrophenyl)-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Me
$$\sim$$
 NO2

Me \sim NO2

Me \sim NO2

RN 118209-91-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-cyclohexyl-2-methyl-5-(2-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118209-92-0 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-hexyl-2-methyl-5-(2-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118209-93-1 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-cyclohexyl-1-(2,4-dichlorophenyl)-2-methyl-5(2-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118209-94-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-dodecyl-2-methyl-5-(2-nitrophenyl)- (9CI) (CA INDEX NAME)

Me-
$$(CH_2)_{11}$$
-NH-C

RN 118209-95-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-hexyl-2-methyl-5-(2-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{Me} \\ \text{Me} \\ \text{(CH2)} \\ \text{5} \\ \text{NH-C} \\ \text{O} \\ \text{O} \\ \text{O} \\ \end{array}$$

RN 118209-97-5 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-cyclohexyl-2-methyl-5-(3-nitrophenyl)-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118209-98-6 HCAPLUS CN 1H-Pyrrole-3-carboxamide, N-dodecyl-2-methyl-5-(3-nitrophenyl)-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Me
$$\sim$$
 NO₂

Me (CH₂)₁₁-NH-C

O

RN 118209-99-7 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-hexyl-2-methyl-5-(3-nitrophenyl)-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Me
$$\sim$$
 NO₂

Me (CH₂)₅-NH-C

 \sim O

RN 118210-01-8 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-cyclohexyl-2-methyl-5-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118210-02-9 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-dodecyl-2-methyl-5-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118210-03-0 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-hexyl-2-methyl-5-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

Me NO₂

$$Me - (CH2)5 - NH - C$$

$$0$$

RN 118210-05-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-cyclohexyl-1-(2,4-dichlorophenyl)-2-methyl-5-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118210-06-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-dodecyl-2-methyl-5-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Cl} & \\ & \text{NO}_2 \\ \text{Me} & \text{N} \\ & \text{Me}^- \text{ (CH}_2)_{11} - \text{NH} - \text{C} \\ & \text{O} \\ \end{array}$$

RN 118210-07-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-hexyl-2-methyl-5-(3-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118228-53-8 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-dodecyl-2-methyl-5-(2-nitrophenyl)- (9CI) (CA INDEX NAME)

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ED Entered STN: 21 Jan 1989

GΙ

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\mathbb{R}^2 \xrightarrow{\mathsf{COR}^1} \mathbb{R}_n
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The synthesis and antifungal activities of the new 1,5-diarylpyrrole derivs. I (R = NO2, Cl; R1 = HNC6H13, HNC12H25, N-methylpiperazinyl, cyclohexylamino; R2 = F, Cl, Br, Me, OMe; n = 1 or 2) are reported. The N-methylpiperazinyl substituent is fundamental to activity. The presence of substituents at the para position of the two Ph rings and the presence of halogen atoms enhance microbiol. activity. The results are discussed in relation to structure-activity relationships.

ACCESSION NUMBER:

1989:20996 HCAPLUS

DOCUMENT NUMBER:

110:20996

TITLE:

Compounds with antibacterial and antifungal activity. Part V. Synthesis and microbiological activity of new

1,5-diarylpyrrole derivatives

AUTHOR (S):

Scalzo, M.; Porretta, G. C.; Chimenti, F.; Bolasco,

A.; Casanova, M. C.; Simonetti, N.; Villa, A.

CORPORATE SOURCE:

Dip. Chim. Tecnol. Sostanze Biol. Attive, Univ. "La

Sapienza", Rome, Italy

SOURCE:

Farmaco, Edizione Scientifica (1988), 43(9), 677-91

CODEN: FRPSAX; ISSN: 0430-0920

DOCUMENT TYPE:

LANGUAGE:

Journal Italian

OTHER SOURCE(S): CASREACT 110:20996
IT 118179-23-0P 118179-24-1P 118179-25-2P
118179-27-4P 118179-28-5P 118179-29-6P
118179-31-0P 118179-32-1P 118179-33-2P

118179-35-4P 118179-36-5P 118179-37-6P 118179-39-8P 118179-40-1P 118179-41-2P

118179-43-4P 118179-44-5P 118179-45-6P 118179-47-8P 118179-48-9P 118179-49-0P

118179-51-4P 118179-52-5P 118179-54-7P

118179-55-8P 118179-56-9P 118179-58-1P

118179-59-2P 118179-60-5P 118179-62-7P

118179-63-8P 118179-64-9P 118179-66-1P 118179-67-2P 118179-68-3P 118179-70-7P

118179-71-8P 118179-72-9P 118179-74-1P

118179-75-2P 118179-76-3P 118209-17-9P 118209-18-0P 118209-19-1P 118210-84-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and antimicrobial activity of)

RN 118179-23-0 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-cyclohexyl-5-(4-fluorophenyl)-2-methyl-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118179-24-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-fluorophenyl)-N-hexyl-2-methyl-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NO}_2 \\ \\ \text{Me} \\ \text{(CH}_2)_5 \\ \text{NH} \\ \text{C} \\ \\ \text{O} \end{array}$$

RN 118179-25-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-dodecyl-5-(4-fluorophenyl)-2-methyl-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{NO}_2 \\ \\ \text{Me} \\ \text{Me} \\ \text{(CH}_2)_{11} \\ \text{NH} \\ \text{C} \\ \\ \text{O} \\ \end{array}$$

RN 118179-27-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-cyclohexyl-5-(4-fluorophenyl)-2-methyl- (9CI) (CA INDEX NAME)

RN 118179-28-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-5-(4-fluorophenyl)-N-hexyl-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Cl} \\ \text{Me} \\ \text{Me} \\ \text{(CH}_2)_5 \\ \text{NH} \\ \text{C} \\ \text{O} \\ \end{array}$$

RN 118179-29-6 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-dodecyl-5-(4-fluorophenyl)2-methyl- (9CI) (CA INDEX NAME)

RN 118179-31-0 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-cyclohexyl-1-(2,4-dichlorophenyl)-5-(4-fluorophenyl)-2-methyl- (9CI) (CA INDEX NAME)

RN 118179-32-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-5-(4-fluorophenyl)-N-hexyl-2-methyl- (9CI) (CA INDEX NAME)

$$C1$$

$$Me \longrightarrow N$$

$$Me - (CH2)5 - NH - C$$

$$0$$

RN 118179-33-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-dodecyl-5-(4-fluorophenyl)-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{Cl} \\ & \text{Me} \\ & \text{N} \\ & \text{Me} \\ & \text{CH}_2)_{11} \\ & \text{NH} \\ & \text{Cl} \\ & \text{Me} \\ & \text{N} \\ & \text{F} \\ & \text{N} \\ & \text{O} \\ & \text{N} \\ & \text{N}$$

RN 118179-35-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-N-cyclohexyl-2-methyl-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118179-36-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-N-hexyl-2-methyl-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118179-37-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-N-dodecyl-2-methyl-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118179-39-8 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1,5-bis(4-chlorophenyl)-N-cyclohexyl-2-methyl-(9CI) (CA INDEX NAME)

RN 118179-40-1 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1,5-bis(4-chlorophenyl)-N-hexyl-2-methyl- (9CI)
(CA INDEX NAME)

Me Cl
$$Me^{-(CH_2)} = NH - C$$
 $Me^{-(CH_2)} = NH - C$ $Me^{-(CH_2)} = NH - C$

RN 118179-41-2 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1,5-bis(4-chlorophenyl)-N-dodecyl-2-methyl(9CI) (CA INDEX NAME)

Me
$$\sim$$
 C1

Me \sim N

Me \sim C1

C1

O

C1

RN 118179-43-4 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-N-cyclohexyl-1-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)

RN 118179-44-5 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-N-hexyl-2-methyl- (9CI) (CA INDEX NAME)

RN 118179-45-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-N-dodecyl-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Cl} \\ \text{Cl} \\ \text{Me} \\ \text{N} \end{array}$$

$$\text{Me} - (\text{CH}_2)_{11} - \text{NH} - \text{C} \\ \parallel \\ \text{O} \\ \end{array}$$

RN 118179-47-8 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-bromophenyl)-N-cyclohexyl-2-methyl-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118179-48-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-bromophenyl)-N-hexyl-2-methyl-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118179-49-0 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-bromophenyl)-N-dodecyl-2-methyl-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118179-51-4 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4-bromophenyl)-1-(4-chlorophenyl)-N-cyclohexyl-2-methyl- (9CI) (CA INDEX NAME)

RN 118179-52-5 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4-bromophenyl)-1-(4-chlorophenyl)-N-hexyl-2-methyl- (9CI) (CA INDEX NAME)

Me-
$$(CH_2)_5$$
-NH-C

RN 118179-54-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-bromophenyl)-N-cyclohexyl-1-(2,4-dichlorophenyl)-2-methyl- (9CI) (CA INDEX NAME)

RN 118179-55-8 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 5-(4-bromophenyl)-1-(2,4-dichlorophenyl)-N-hexyl-2-methyl-(9CI) (CA INDEX NAME)

RN 118179-56-9 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4-bromophenyl)-1-(2,4-dichlorophenyl)-N-dodecyl-2-methyl- (9CI) (CA INDEX NAME)

$$C1$$
 Me
 N
 $Me^{-(CH_2)}_{11}-NH^{-C}$
 0

RN 118179-58-1 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-cyclohexyl-2-methyl-5-(4-methylphenyl)-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118179-59-2 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-hexyl-2-methyl-5-(4-methylphenyl)-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Me
$$\sim$$
 \sim \sim Me \sim Me \sim Me \sim \sim Me \sim \sim Me

RN 118179-60-5 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-dodecyl-2-methyl-5-(4-methylphenyl)-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Me
$$\sim$$
 Me \sim Me \sim Me \sim Me

RN 118179-62-7 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-cyclohexyl-2-methyl-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 118179-63-8 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-hexyl-2-methyl-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)

Me
$$\sim$$
 N Me Me \sim C1 \sim Me Me \sim C1 \sim Me \sim Me \sim O

RN 118179-64-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-dodecyl-2-methyl-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 118179-66-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-cyclohexyl-1-(2,4-dichlorophenyl)-2-methyl-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 118179-67-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-hexyl-2-methyl-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)

$$C1$$
 Me
 N
 Me
 N
 Me
 N
 Me
 N
 Me
 N
 Me

RN 118179-68-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-dodecyl-2-methyl-5-(4-methylphenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{C1} \\ \text{Me} \\ \text{Me} \\ \text{(CH2)} \\ \text{11} \\ \text{NH} \\ \text{C} \\ \text{O} \\ \end{array}$$

RN 118179-70-7 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-cyclohexyl-5-(4-methoxyphenyl)-2-methyl-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118179-71-8 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, N-hexyl-5-(4-methoxyphenyl)-2-methyl-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

Me-
$$(CH_2)_5$$
-NH-C

RN 118179-72-9, HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-dodecyl-5-(4-methoxyphenyl)-2-methyl-1-(4-nitrophenyl)- (9CI) (CA INDEX NAME)

RN 118179-74-1 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-cyclohexyl-5-(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)

RN 118179-75-2 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-hexyl-5-(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)

Me-
$$(CH_2)_5$$
- NH- C OMe

RN 118179-76-3 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(4-chlorophenyl)-N-dodecyl-5-(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)

Me-
$$(CH_2)_{11}$$
- NH- C OMe

RN 118209-17-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, N-cyclohexyl-1-(2,4-dichlorophenyl)-5-(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)

RN 118209-18-0 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-hexyl-5-(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Cl} \\ \text{Me} \\ \text{Me} \\ \text{(CH}_2)_5 - \text{NH-C} \\ \text{O} \\ \end{array}$$

RN 118209-19-1 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 1-(2,4-dichlorophenyl)-N-dodecyl-5-(4-methoxyphenyl)-2-methyl- (9CI) (CA INDEX NAME)

RN 118210-84-7 HCAPLUS
CN 1H-Pyrrole-3-carboxamide, 5-(4-bromophenyl)-1-(4-chlorophenyl)-N-dodecyl-2-methyl- (9CI) (CA INDEX NAME)

L4 ANSWER 24 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 12 May 1984

GI

AB The title compound (I) was prepared by reaction of o-H2NC6H4CONH2 with SOC12.

I reacted with 2-amino-1,4,5-triphenyl-3-pyrrolecarboxamide to give pyrrolothiadiazinone II. Chlorination of I with SCl2 or SO2Cl2 gave

2,5-H2NClC6H3CONH2. Bromination of I with Br at 0° gave

2,5-H2NBrC6H3CONH2 and at 20° gave 2,3,5-H2NBr2C6H2CONH2. I and

Me2CO gave quinazoline III.

ACCESSION NUMBER: 1981:407231 HCAPLUS

DOCUMENT NUMBER:

95:7231

TITLE:

Synthesis and reactions of 1,3-didehydro-2,1,3-

benzothiadiazin-4-one

AUTHOR (S):

Eger, Kurt

CORPORATE SOURCE:

Pharm. Inst., Univ. Bonn, Bonn-Endenich, 5300, Fed.

Rep. Ger.

SOURCE:

Archiv der Pharmazie (Weinheim, Germany) (1981),

314(2), 176-80

CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE:

LANGUAGE:

Journal German

OTHER SOURCE(S):

CASREACT 95:7231

IT 56023-01-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with didehydrobenzothiadiazinone, pyrrolothiadiazinone

derivative from)

RN 56023-01-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-amino-1,4,5-triphenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 25 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 12 May 1984

GΙ

AB Thiadiazines I (X = PhCH2N, PhCH2CH2N, cyclohexylimino, Me(CH2)5N, MeN, Me2CHN, Me2N(CH2)3N, O) were prepared by treating the amides II (R = Ph)

with SOCl2, SCl2, or S2Cl2. The thiadiazine oxides III [R = Me, R2 = (CH2)4] were prepared by reaction of II (X = S) with SOCl2. II were prepared

by hydrolysis of the corresponding nitriles.

ACCESSION NUMBER: 1981:208819 HCAPLUS

DOCUMENT NUMBER: 94:208819

TITLE: Synthesis of bicyclic 1,2,6-thiadiazines

AUTHOR(S): Offermann, Wolfgang; Eger, Kurt; Roth, Hermann J. CORPORATE SOURCE: Pharm. Inst., Univ. Bonn, Bonn-Endenich, 5300, Fed.

Rep. Ger.

SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1981),

314(2), 168-75

CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal LANGUAGE: German

OTHER SOURCE(S): CASREACT 94:208819

IT 56023-01-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(cyclocondensation of, with sulfur)

RN 56023-01-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-amino-1,4,5-triphenyl- (9CI) (CA INDEX NAME)

IT 77651-28-6P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and cyclization with disulfur dichloride)

RN 77651-28-6 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-amino-1-cyclohexyl-4,5-diphenyl- (9CI) (CA INDEX NAME)

$$H_2N$$
 H_2N
 Ph
 H_2N
 O

L4 ANSWER 26 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 12 May 1984

GI

AB The title pyrrole derivs. (I; R, R1 = CH2CO2Et, OEt; CH2CO2H, OH; $\alpha\text{-naphthyl}$, OEt; $\alpha\text{-naphthyl}$, NHNH2; o-tolyl, OEt; $\alpha\text{-naphthyl}$, OH; o-tolyl, OH; o-tolyl, NHNH2; o-tolyl, NHN:CHPh) were prepared by Knorr-Paal synthesis. Thus, 2 g II and 1 g $\alpha\text{-naphthylamine}$ in 1,4-dioxane were refluxed 3 h and the oily residue refluxed in 20% KOH-EtOH to give 66% I (R = $\alpha\text{-naphthyl}$, R1 = OH).

II

ACCESSION NUMBER: 1981:174785 HCAPLUS

DOCUMENT NUMBER: 94:174785

TITLE: Synthesis of sterically hindered polysubstituted

pyrroles

AUTHOR(S): Hua, Wen-Ting

CORPORATE SOURCE: Dep. Chem., Peking Univ., Peking, Peop. Rep. China

SOURCE: Huaxue Tongbao (1980), (11), 662-4

CODEN: HHTPAU; ISSN: 0441-3776

DOCUMENT TYPE: Journal LANGUAGE: Chinese

IT 77412-53-4P 77412-54-5P 77418-98-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 77412-53-4 HCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 2-methyl-1-(2-methylphenyl)-5-(2-naphthalenyl)-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)

Young, Shawquia, Page 133

RN 77412-54-5 HCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 2-methyl-1-(2-methylphenyl)-5-(2-naphthalenyl)-, hydrazide (9CI) (CA INDEX NAME)

RN 77418-98-5 HCAPLUS

CN 1H-Pyrrole-3-carboxylic acid, 2-methyl-1-(1-naphthalenyl)-5-(2-naphthalenyl)-, hydrazide (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ Me & & N \\ & & \\ H_2N-NH-C \\ & & \\ O \end{array}$$

ANSWER 27 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 12 May 1984

GI

L4

AB The pyrrolothiadiazine I was formed by treating the pyrrolecarboxamide II

(R = CONH2, R1 = NH2) with SOCl2 in dioxane at 90°, in THF at

20°, or in DMF at 0°. The same reaction in DMF 30°

gave I (R = CN, R1 = N:CHNMe2) and at 80-100° gave III (X = CHNMe2)

in acetone at 20-30° III (X = CMe2) was obtained.

ACCESSION NUMBER: 1977:55398 HCAPLUS

DOCUMENT NUMBER: 86:55398

TITLE: Formation of a novel ring system:

pyrrolo[2,3-e]-thiadiazine

AUTHOR(S): Kim-Su, Myungeun; Eger, Kurt; Roth, Hermann J.

CORPORATE SOURCE: Pharm. Inst., Univ. Bonn, Bonn, Fed. Rep. Ger. SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1976),

309(9), 721-4

CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: Journal LANGUAGE: German

IT 56023-01-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with thionyl chloride, solvent effect on)

RN 56023-01-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-amino-1,4,5-triphenyl- (9CI) (CA INDEX NAME)

L4 ANSWER 28 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 12 May 1984

GI For diagram(s), see printed CA Issue.

AB The title ring systems (I, X = N, S) were obtained by hydrolyzing the pyrrole II (R = CN) with polyphosphoric acid-H3PO4 and cyclizing II (R = CONH2) with NaNO2 or SOCl2. Hydrolysis of II (R = CN) with 100% H3PO4

gave II (R = CO2H).

ACCESSION NUMBER: 1975:428198 HCAPLUS

DOCUMENT NUMBER: 83:28198

TITLE: Two new rings systems. Pyrrolo[2,3-d]azimide and

pyrrolo[2,3-e]thiadiazine

AUTHOR(S): Roth, H. J.; Eger, K.

CORPORATE SOURCE: Pharm. Inst., Univ. Bonn, Bonn, Fed. Rep. Ger. SOURCE: Archiv der Pharmazie (Weinheim, Germany) (1975),

308(3), 186-9

CODEN: ARPMAS; ISSN: 0365-6233

DOCUMENT TYPE: LANGUAGE:

Journal German

IT 56023-01-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and cyclization of, with nitrite or thionyl chloride)

RN 56023-01-9 HCAPLUS

CN 1H-Pyrrole-3-carboxamide, 2-amino-1,4,5-triphenyl- (9CI) (CA INDEX NAME)

AB

L4 ANSWER 29 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

ED Entered STN: 16 Dec 2001

GI For diagram(s), see printed CA Issue.

1,2,5-Triphenyl-3-pyrrolecarboxylic acid and SOCl2 give the chloride (I) as a red resin; the anilide, from I and PhNH2 in boiling C6H6, m. 171°; Me ester, m. 156-7°. I and C6H6 with AlCl3 give 1,2,4-triphenyl-3-benzoylpyrrole, yellow, m. 238°. PhCH2COCH2CO2Et and PhCOCH2Br with Na give Et γ -phenyl- α -phenacylacetoacetate (II) which with NH3 in EtOH yields Et γ -phenyl- α -phenacylβ-aminocrotonate, m. 166-7°; N H2SO4 gives 5-phenyl-2-benzyl-3-pyrrolecarboxylic acid, m. 181°; Et ester, m. 137°; the acid chloride could not be prepared II and PhNH2 in AcOH give 1,5-diphenyl-2-benzyl-3-pyrrolecarboxylic acid, m. 191°; Et ester, m. 100-1°; again the acid chloride could not be prepared PhCH2COCO2Et and PhNMeNH2 in 2 N HCl give 1-methyl-3-phenyl-2indolecarboxylic acid (IIA), m. 197-8°; chloride (III), b0.5 180°, m. 100°. III and C6H6 with Al 13 give 1-methyl-1'-oxoindeno[2',3',2,3]indole (IV), reddish brown, m. 147-8°; 2,4-dinitrophenylhydrazone, brownish violet, m. 313-14°. With concentrated H2SO4 IIA gives 1-methyl-3-phenylindole, m. 65°. Et benzoylacetate asymmethylphenylhydrazone, yellow, 128°; HCl in EtOH gives the Et ester, m. 97° (picrate, yellow, m. 137-8°), of 1-methyl-2-phenyl-3-indolecarboxylic acid, m. 201-2°; the chloride and C6H6 with AlCl3 give 1-methyl-2-phenyl-3-benzoylindole, yellow, m. 130°; 2,4-dinitrophenylhydrazone, deep red, m. 269°. 1-Methyl-3-benzyl-2-indolecarboxylic acid, m. 194°; the chloride, yellow, m. 117-18°; AlCl3 and C6H6 give 9-methyl-2,3-benzo-1-oxo-1,4-dihydrocarbazole (V), yellow, m. 215-16°. 3-Phenyl-2indolecarboxylic acid, m. 186°; chloride, pale yellow, m. 164° (decomposition), which then does not m. at 360°; the chloride on heating at 175-80° or with AlCl3 in PhNO2 gives 3',3''-diphenyl-1,2,4,5,1',2',1'',2''-diindolo-3,6-diketopiperazine (VI), yellow powder. VI heated with C5H5N or N2H4.H2O at 200° gives 3-phenyl-2-indolecarboxylic hydrazide, m. 227°; benzylidene compound, m. 237°. Phenylpyruvic acid 4-toluylhydrazone, yellow, m. 145-6°; alc. HCl gives 5-methyl-3-phenyl-2-indolecarboxylic acid,